PASSION FOR KNOWLEDGE

THE WORKSHOPS

28 SEPT-1 OCT 2010
Donostia-San Sebastian

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Celebrating **10 years**

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PREFACE

Dear Colleague,

On April 27th 2000, Donostia International Physics Center (DIPC) was officially inaugurated as a center fostering exchange and creativity between scientists from the world around. Since its creation, DIPC has been an open institution committed to the progress of science and knowledge. After ten years of activity, we can proudly say that our objectives are being accomplished. More than 1200 researchers have visited DIPC so far and more than 6000 have attended scientific meetings organized by DIPC. But, more important, many of these scientists have found in DIPC a fertile ground to develop their research, are now frequent visitors of the center, and have become members and ambassadors of a DIPC community that spreads worldwide.

With Passion for Knowledge, we want to celebrate the first ten years of the existence of DIPC. We also want to begin a new decade that we hope will be even more exciting than the past. Passion for Knowledge is a fest that brings together world leading scientists and other humanists from different disciplines, cultures and thinking, driven by a love of knowledge for its own sake. Passion for Knowledge is a large event split into three main programs: “The Workshops”, “The Lectures” and “The City”.

“The Workshops” are a key element in Passion for Knowledge. Scientific research is the soul of DIPC. Therefore, an event such as Passion for Knowledge necessarily had to include scientific meetings covering the main lines of research at DIPC. Four scientific workshops will run in parallel and we encourage you to share your time among them.

We also encourage you to actively participate in further activities included in the program of Passion for Knowledge. In “The Lectures”, world-leading experts will speak about the challenges and implications of their work. “The Lectures” will combine scientific rigor and entertainment to awake the curiosity and critical thinking of the public at large. “The City” includes outreach activities (encounters, exhibitions, contests, etc.) across the city of Donostia-San Sebastian, emphasizing the role of science as an essential part of culture.

We hope that you enjoy your stay. Thank you for sharing this Passion for Knowledge with us.

Pedro M. Echenique
Conference Chairman

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CENTER

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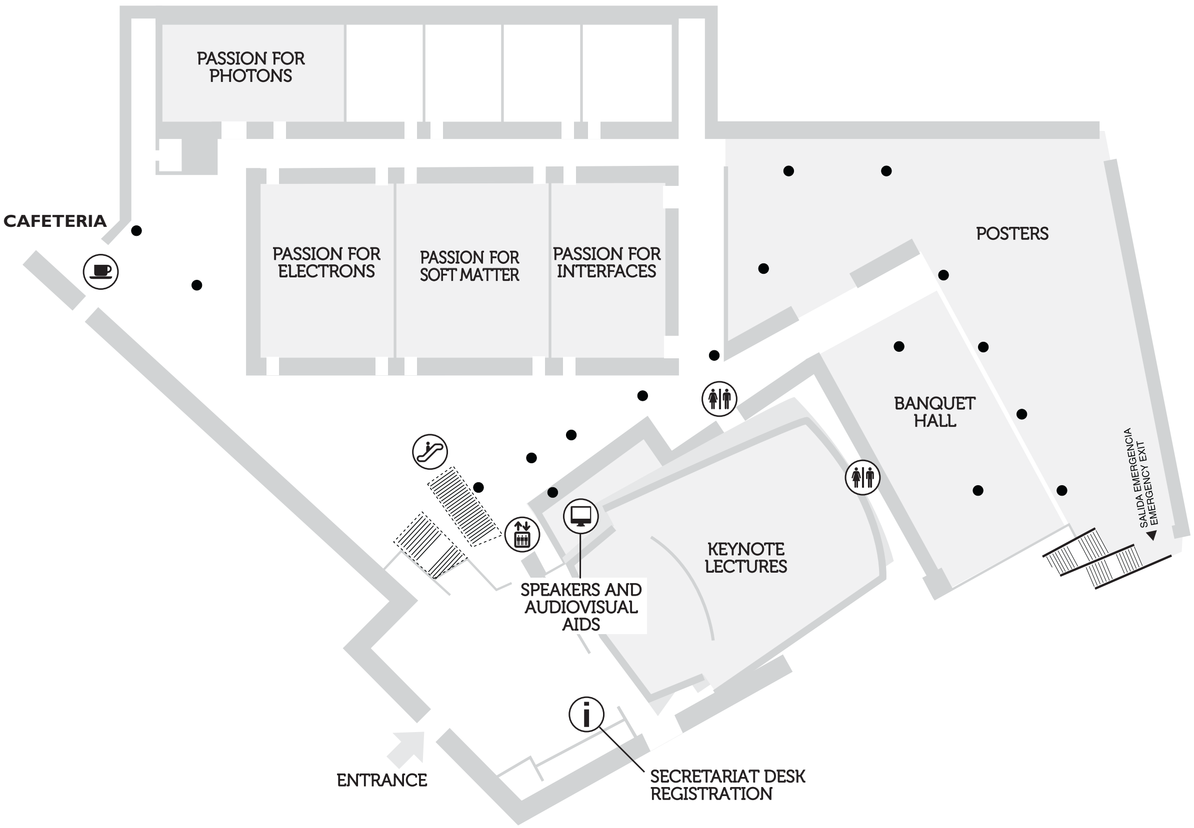
PLAN
KURSAAL CONFERENCE CENTER



THE WORKSHOPS

PROGRAM

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10:50 - 11:30	COFFEE BREAK			
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		▪ KEYNOTE LECTURE CHAIRMAN: Prof. Martin Weinelt (Free University Berlin, Germany)		
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		▪ INVITED LECTURES / ORAL CONTRIBUTIONS CHAIRMAN: Prof. Martin Weinelt (Free University Berlin, Germany)		
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10:35	11:05	**Prof. Fernando MARTÍN** (Universidad Autónoma de Madrid, Madrid, Spain) *Electron Localization following Attosecond Molecular Photoionization of* H_2	I-10	67
11:05	11:25	**Prof. Dietrich MENZEL** (Fritz Haber Institute of the MPS, Berlin. Physik-Dept, Techn. University of Munich, Munich, Germany) *NO photochemistry on silver nanoparticles by nanosecond vs. femtosecond excitation*	0-07	80
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		▪ INVITED LECTURES / ORAL CONTRIBUTIONS CHAIRMAN: Dr. Philip Hofmann (University of Aarhus, Denmark)		
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15:30	15:50	**Dr. Andrey KAZANSKY** (V A Fock Institute of Physics, St. Petersburg, Russia) *Some aspects of the theory of streaking experiments with sub-femtosecond pulses on solids.*	0-04	77
15:50	16:10	**Dr. Christoph LEMELL** (Vienna University of Technology, Vienna, Austria) *Modeling XUV-NIR streaking experiments at metal surfaces*	0-05	78

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		■ INVITED LECTURES / ORAL CONTRIBUTIONS CHAIRMAN: Prof. Geert-Jan Kroes (Leiden University, Netherlands)		
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15:30	15:50	**Dr. Pascal LARREGARAY** (CNRS/ Université Bordeaux1, Talence, France) *Theoretical investigation of the Eley–Rideal recombination of nitrogen on Tungsten(100)*	0-14	139
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		▪ NOVEL MATERIALS CHAIRMAN: Prof. José A. Pomposo (CFM, UPV/EHU-CSIC & IKERBASQUE, Spain)		
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		▪ INVITED LECTURES / ORAL CONTRIBUTIONS CHAIRMAN: Prof. Hrvoje Petek (University of Pittsburgh, USA)		
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11:30	12:15	**Prof. Dieter RICHTER** (Forschungszentrum Juelich GmbH, Juelich, Germany) *Soft Matter and Life Sciences: Research with Neutrons*	K-03	189
		▪ INVITED LECTURES / ORAL CONTRIBUTIONS CHAIRMAN: Prof. Amand Lucas (Univ. Notre-Dame de la Paix, Namur, Belgium)		
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12:50	13:20	**Prof. Angel RUBIO** (Nano–Bio Spectroscopy Group, Dept. Física de Materiales, UPV/EHU. ETSF , Donostia-San Sebastian, Spain) *First principle modeling of the excited state properties of complex nanostructures and biomolecules: a TDDFT and Many-Body perturbation theory approach*	I-15	72
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		▪ KEYNOTE LECTURE CHAIRMAN: Dr. Javier Aizpurua (CFM and DIPC, San Sebastián, Spain)		
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		▪ INVITED LECTURES / ORAL CONTRIBUTIONS CHAIRWOMAN: Prof. Maki Kawai (RIKEN, Wako, Japan)		
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		▪ INVITED LECTURES / ORAL CONTRIBUTIONS CHAIRMAN: Prof. Aart Kleyn (FOM Institute, Nieuwegein, Netherlands)		
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12:50	13:20	**Dr. Fabio BUSNENGO** (Instituto de Física de Rosario, IFIR-CONICET. Universidad Nacional de Rosario, Rosario, Argentina) *Structure of self-assembled monolayers of alkylthiolates on Au(111) and Ag(111): a comparative study based on Density Functional and post Hartree-Fock calculations*	I-18	121
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		■ KEYNOTE LECTURE CHAIRMAN: Dr. Javier Aizpurua (CFM and DIPC, San Sebastián, Spain)		
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		■ EMERGING PROPERTIES CHAIRMAN: Prof. Lars Börjesson (Chalmers University of Technology, Sweden)		
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11:30	12:15	**Prof. Dieter RICHTER** (Forschungszentrum Juelich GmbH, Juelich, Germany) *Soft Matter and Life Sciences: Research with Neutrons*	K-03	189
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		■ KEYNOTE LECTURE CHAIRMAN: Dr. Javier Aizpurua (CFM and DIPC, San Sebastián, Spain)		
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		■ NANOANTENNAS CHAIRMAN: Dr. Rainer Hillenbrand (CIC Nanogune, San Sebastián, Spain)		
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10:20	10:50	**Dr. Garnett W. BRYANT** (Atomic Physics Div. and Joint Quantum Institute, National Institute of Standards and Technology, Gaithersburg - MD, USA) *Photonics with nanohybrids*	I-47	274
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		■ CONCEPTS IN OPTICS CHAIRMAN: Prof. F. Javier García de Abajo (Insituto Optica CSIC, Madrid, Spain)		
12:20	12:50	**Prof. John B. PENDRY** (Imperial College London, London, UK) *Transformation Optics at Optical Frequencies*	I-57	285
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		▪ INVITED LECTURES / ORAL CONTRIBUTIONS CHAIRMAN: Prof. Ulrich Höfer (University of Margburg, Germany)		
09:50	10:20	**Prof. Hrvoje PETEK** (University of Pittsburgh, Pittsburgh - KS, USA) *Imaging the femtosecond time scale correlated electron-nuclear dynamics in surface photodesorption*	I-12	69
10:20	10:50	**Prof. Evgueni CHULKOV** (DIPC - Donostia International Physics Center, Donostia-San Sebastian, Spain) *Decay mechanisms of electron excitations on clean and nanostructured metal surfaces*	I-03	60
10:50	11:10	**Dr. Andreas HEIDENREICH** (Universidad del País Vasco - UPV/EHU, Donostia-San Sebastian. IKERBASQUE, Bilbao, Spain) *Laser pulse length dependence of electron and nuclear dynamics in Coulomb explosions of xenon clusters*	0-03	76
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		▪ INVITED LECTURES / ORAL CONTRIBUTIONS CHAIRMAN: Prof. Mario Rocca (University of Genoa, Italy)		
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12:10	12:40	**Prof. Branko GUMHALTER** (Institute of Physics, Zagreb, Croatia) *Ultrafast electron dynamics in pump-probe spectroscopies of surfaces: from transient excitonic to quasi-stationary polaronic states*	I-05	62
12:40	13:10	**Prof. Jose Maria PITARKE** (nanoGUNE, Donostia-San Sebastian, Spain) *The asymptotic behavior of the Kohn-Sham potential of Density-Functional Theory at metal surfaces*	I-13	70
13:10	13:30	**Prof. Vladimir NAZAROV** (RCAS, Academia Sinica, Taipei, Taiwan) *Performance of the exchange-correlation kernel of time-dependent density-functional theory derived from LDA to current-density functional theory*	0-08	81

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15:30	15:50	**Prof. Amand LUCAS** (FUNDP, NAMUR, Belgium. DIPC - Donostia International Physics Center, Donostia-San Sebastian, Spain) *Plasmon tsunami on* C_{60} *caused by electron transfer to a highly charged ion*	0-06	79
15:50	16:10	**Dr. Leonor CHICO** (ICMM-CSIC, Madrid, Spain) *Interface states in carbon nanotube junctions: rolling up graphene*	0-01	74
16:10	16:30	**Dr. Jin ZHAO** (University of Pittsburgh, Pittsburgh - KS, USA) *The Electronic Structure Graphane and Graphane Nanostructures from Ab Initio Theory*	0-10	83
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10:20	10:50	**Prof. Pietro GAMBARDELLA** (Centre d´Investigació en Nanociència i Nanotecnologia, ICN-CSIC. ICREA, Bellaterra, Spain) *Spin-spin and spin-orbital coupling effects at metallic interfaces*	I-19	122
10:50	11:10	**Dr. Lucia VITALI** (IKERBASQUE. CFM, UPV/EHU, Donostia-San Sebastian, Spain. Max-Planck-Institut for Solid State Physics, Stuttgart, Germany) *Potential barrier mapping at metal-organic nanocontacts*	0-20	145
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12:10	12:40	**Dr. Nicolás LORENTE** (Centre d´Investigació en Nanociència i Nanotecnologia, ICN-CSIC, Bellaterra, Spain) *Mixed-valency signature in vibrational inelastic electron tunneling spectroscopy*	I-24	127
12:40	13:10	**Prof. José Ignacio PASCUAL** (Institut für Experimentalphysik, Freie Universität, Berlin, germany) *Charging and electric field gating individual molecules at a hybrid metal-organic interface*	I-27	130
13:10	13:30	**Dr. Aitor MUGARZA** (Centre d´Investigació en Nanociència i Nanotecnologia, ICN-CSIC, Bellaterra, Spain) *Exotic Kondo effect in metalorganic complexes controlled by ion-substrate interaction*	0-18	143

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16:10	16:30	**Dipl. Phys. Gerson METTE** (Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität Marburg, Marburg, Germany) *Time-resolved investigation of laser-induced diffusion by optical second-harmonic microscopy*	0-15	140
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10:50	11:10	**Prof. Vladimir NOVIKOV** (The University of Tennesse, Department of Chemistry, Knoxville - TN, USA) *Influence of pressure on fast relaxation in glass-forming materials*	O-30	214
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12:40	13:10	**Dr. Reidar LUND** (DIPC - Donostia International Physics Center, Donostia-San Sebastian, Spain) *Morphological Transition Kinetics in Amphiphilic Block Copolymer Micelles Explored by Small-angle Scattering in the millisecond range*	I-39	197
13:10	13:30	**Prof. Soeren TOXVAERD** (Roskilde University, Roskilde, Denmark) *Crystallization of supercooled nanodroplets*	O-31	215

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15:00	15:30	**Dr. Ángel MORENO** (Centro de Física de Materiales, CSIC - UPV/EHU, Donostia-San Sebastian, Spain) *Computer simulations of polymer blends: from structural relaxation to chain dynamics*	I-40	198
15:30	15:50	**Dr. Jörg BASCHNAGEL** (Institut Charles Sadron, Strasbourg, France) *Deviations from Chain Ideality in Polymer Melts*	O-21	205
15:50	16:10	**Dr. Apostolos KYRITSIS** (National Technical University of Athens, Athens, Greece) *Dynamic heterogeneity in binary poly(ethyl acrylate) /p-xylene mixtures*	O-24	208
16:10	16:30	**Dr. Nigel CLARKE** (Durham University, Durham, UK) *Dynamics in polymer nanocomposites*	O-22	206
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		■ ELECTRONS AND PHOTONS CHAIRMAN: Prof. Peter Nordlander (Rice University, Houston, USA)		
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10:20	10:50	**Prof. Javier GARCÍA DE ABAJO** (Instituto de Óptica,CSIC, Madrid, Spain) *Photons and electrons team up*	I-49	277
10:50	11:10	**Dr. Alejandro REYES-CORONADO** (IESL-FORTH , Heraklion, Greece) *Moving plasmonic nanoparticles through electromagnetic forces induced by fast electron beams*	O-45	303
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12:10	12:40	**Prof. Mark I. STOCKMAN** (Department of Physics and Astronomy, Georgia State University, Atlanta - GA, USA) *Trends in Nanoplasmonics: Ultrasmall, Ultrafast, Ultrastrong*	I-60	288
12:40	13:00	**Dr. Otto MUSKENS** (University of Southampton, Southampton, UK) *Active plasmonic nanoantennas for optical switching*	O-43	301
13:00	13:20	**Dr. Riccardo SAPIENZA** (ICFO - The Institute of Photonic Sciences, Castelldefels, Spain) *LDOS fluctuations probed by single-molecule spectroscopy in random and periodic media*	O-47	305

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15:30	15:50	**Dr. Damien RIEDEL** (CNRS, ORSAY, France) *A scanning tunneling microscope as a tunable nanoantenna for atomic scale control of optical-field enhancement*	O-46	304
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16:10	16:30	**Dr. Amador MENÉNDEZ VELÁZQUEZ** (ITMA, CINN, Asturias, Spain. Dept. of Electrical Engineering and Computer Science, MIT, Cambridge - MA, USA) *Improving the efficiency of luminiscent solar concentrators*	O-41	299
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10:00	10:30	**Prof. Juan José SÁENZ** (Moving Light and Electrons (Mole) Group, Dept. Física de la Materia Condensada, Universidad Autónoma, Madrid, Spain) *Resonant Optical Forces on Metallic and Dielectric Nanoparticles*	I-59	287
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11:45	12:15	**Prof. Mikael KÄLL** (Division of Bionanophotonics, Department of Applied Physics Chalmers University of Technology, Göteborg, Sweden) *Nanoplasmonic sensing: refractive index, SERS and optical forces*	I-53	281
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15:50	16:10	**Mr. Bjoern NIESEN** (IMEC vzw, Leuven, Belgium) *Interactions of excitons with localized surface plasmons in organic semiconductor-metal nanoparticle thin-films*	O-44	302
16:10	16:30	**Dr. Antonio I. FERNÁNDEZ DOMÍNGUEZ** (Imperial College London, London, UK) *Kissing spheres: broadband response and superfocusing properties*	O-35	293

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	Mr. Peter AMANN (Institute of Physical Chemistry, University of Innsrbuck, Innsbruck, Austria) *Is the surface of Pd(110) magnetic?*	P-003	86
	Dr. Andres AYUELA (Centro de Física de Materiales, CSIC - UPV/EHU, Donostia-San Sebastian, Spain) *Interface States in Carbon Nanotube Junctions: Rolling up graphene*	P-004	87
	Dr. Andres AYUELA (Centro de Física de Materiales, CSIC - UPV/EHU, Donostia-San Sebastian, Spain) *Interface States in Carbon Nanotube Junctions: Rolling up graphene*	P-005	88
	Dr. Kuntala BHATTACHARJEE (Max Planck Institute of Microstructure Physics, Halle, Germany) *LT-STS study of atomic nanowires on Cu_3N/Cu(110) surface*	P-006	89
	Mr. Marco BIANCHI (Univesity of Aarhus, Aarhus, Denmark) *Fermi surface and electronic structure of Sb(110)*	P-007	90
	Dr. Helga BOEHM (Theoretical Physics, JKU, Linz, Austria) *Dynamic Correlations of the 3D and 2D Electron Liquid*	P-008	91
	Mr. Michael CAMINALE (Department of Physics, University of Genoa, Genoa, Italy) *Growth of magnetic nanostructures on self-organized substrates*	P-009	92
	Mr. Cheng - Tien CHIANG (Max Planck Institute of Microstructure Physics, Halle, Germany) *Unoccupied quantum well states in ultrathin cobalt films studied by two-photon photoemission*	P-010	94
	Dr. Vito DESPOJA (DIPC - Donostia International Physics Center, Donostia-San Sebastian, Spain) *Some quantum mechanical aspects of frictional force between parallel metallic slabs*	P-011	95

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	Ms. Johanna FUKS (Universidad del País Vasco - UPV/EHU, Donostia-San Sebastian, Spain) *Rabi oscillations in Time-dependent Density Functional Theory*	P-014	98
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	Dr. Rene GAUDOIN (University of Vienna, Vienna, Austria) *k-space based finite-size corrections for Quantum Monte Carlo calculations*	P-016	100
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	Mr. Christopher ZAUM (Institut für Festkörperphysik, Abteilung ATMOS, Gottfried Wilhelm Leibniz Universität, Hannover, Germany) *Local investigation of fs-laser induced defects on Ag(100)*	P-029	114
	Mr. Xabier ZUBIZARRETA (Univ. del País Vasco - UPV/EHU, DIPC - Donostia International Physics Center, Donostia-San Sebastian, Spain) *Ab initio study on bulk Pb dielectric response and quasiparticle inelastic lifetime.*	P-031	115
	Mr. Asier ZUGARRAMURDI (Uni. del País Vasco - UPV/EHU, Leioa, Centro de Física de Mat., CSIC-UPV/EHU, Donostia-San Sebastian, Spain) *Lifetime of quantum well states in Pb overlayers*	P-032	116

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	Ms. Sara BARJA (Universidad Autónoma de Madrid, Instituto Madrileño de Estudios Avanzados en Nanociencia, IMDEA-Nanociencia, Madrid, Spain) *Field Emission Resonances on periodically rippled graphene*	P-037	150
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	Dr. Geethalakshmi K.RANGASWAMY (CFM, CSIC - UPV/EHU, MPC, DIPC - Donostia International Physics Center, Donostia-San Sebastian, Spain) *Probing the scattering of N_2 from W(110) surface with different exchange-correlation functionals*	P-053	166
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	Dr. Cédric MASTAIL (CNRS; LAAS / Université de Toulouse ; UPS , INSA , INP, ISAE ; LAAS / CEA, DAM, DIF, Toulouse, France) *Oxide nuclei propagation through the channel separating two dimer rows onto silicon(100) surface*	P-057	170
	Dr. Manfred MATENA (DIPC - Donostia International Physics Center, Donostia-San Sebastian, Spain) *Molecule-substrate interactions of ordered surface structures*	P-058	171
	Dr. Luis M. MOLINA (Universidad de Valladolid, Valladolid, Spain) *Ab initio studies of propene epoxidation at noble metal nanocatalysts*	P-059	172
	Dr. Miguel Ángel MUÑOZ-MÁRQUEZ (Centro de Física de Materiales, CSIC - UPV/EHU, Donostia-San Sebastian, Spain) *Permanent magnetism in phosphine- and chlorine-capped gold clusters and nanoparticles*	P-060	173
	Ms. Maider ORMAZA (Centro de Física de Materiales, CSIC - UPV/EHU, Donostia-San Sebastian, Spain) *Rare Earth /gold surface compounds*	P-061	174
	Prof. Enrique ORTEGA (Universidad del País Vasco - UPV/EHU, Donostia-San Sebastian, Spain) *Surface states and structural stability in step lattices investigated with curved crystals*	P-062	175
	Ms. Irene PALACIO (Universidad Autónoma de Madrid. Departamento de Física de Materiales, Madrid, Spain) *Surface defects activate new reaction paths: formate formation during methanol decomposition on Ru(0001)*	P-063	176
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	Dr. Frederik SCHILLER (Centro de Física de Materiales, CSIC - UPV/EHU, Donostia-San Sebastian, Spain) *Superlattice bands in tunable dislocation networks: structural/electronic interplay*	P-068	181
	Mr. Daniele STRADI (Autonomous University of Madrid. IMDEA Nanoscience, Madrid, Spain) *Scattering of Vibrationally Excited* H_2 *from Metal Surfaces at Grazing Incidence*	P-069	182
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	Dr. Fabienne BARROSO-BUJANS (Centro de Física de Materiales, CSIC - UPV/EHU, Donostia-San Sebastian, Spain) *Intercalated molecules of variable sizes into graphite oxide at the sub-nanometric scale: confinement effects on the dynamics and crystallization.*	P-076	218
	Prof. Josef BARTOS (Polymer Institute of SAS, Bratislava, Slovakia) *Atomistic and molecular probing of amorhous polymers in relation to neutron scattering and dielectric relaxation dynamics: Poly(vinylmethyl ether)*	P-077	219
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	Dr. Pablo BLANCO (Forschungszentrum Juelich GmbH, Juelich, Germany) *Investigation of fd-virus in a temperature gradient*	P-080	222
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	Dr. Martin BRODECK (IFF- Forschungszentrum Juelich GmbH, Juelich, Germany) *Computer simulations and neutron scattering experiments on the polymer blend PEO/PMMA*	P-082	224
	Dr. Remi BUSSELEZ (DIPC - Donostia International Physics Center, Donostia-San Sebastian, Spain) *Dynamics of hydration water in a Polymer system*	P-083	225
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	Ms. Caroline CRAUSTE-THIBIERGE (Laboratoire Léon Brillouin, Gif-sur-Yvette, France) *Stable vs normal glass: to a better understanding of aging in glasses.*	P-086	228
	Dr. Alessio DE FRANCESCO (CNR-IOM-OGG, Grenoble, France) *Possible Natural Tuning of Protein and Water Dynamics in the Terahertz Window*	P-087	229
	Ms. Lourdes DEL VALLE-CARRANDI (CFM, CSIC - UPV/EHU. Dept. de Física de Materiales. UPV/EHU. Donostia-San Sebastian. Spain) *Nanocomposites based on Nanostructured diblock copolymers and Nanoparticles*	P-088	230
	Mr. Florian EVERS (Technische Universität Dortmund, Dortmund, Germany) *Effect of osmolytes and Hofmeister salts on protein adsorption*	P-089	231
	Dr. F. FARIA (University of Aveiro, Aveiro, Portugal) *Lignin/carbon nanotubes composites with low percolation threshold*	P-090	232
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	Mr. Mathieu LEOCMACH (University of Tokyo, Tokyo, Japan) *Local and medium range structures in supercooled colloidal liquids and their link with dynamics: confocal microscopy study.*	P-098	240
	Dr. Marco MACCARINI (Institut Laue-Langevin, Grenoble, France) *Structure and dynamics of polymer coated gold nanoparticles*	P-099	241
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	Dr. Jonathan NICKELS (Dept. of Chemistry, Univ. Tennesse, Knoxville. Chemical Sciences Div., Oak Ridge National Laboratory, Oak Ridge - TN, USA) *Role of Methyl Groups in Dynamics and Function of Biomolecules*	P-104	246
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	Mr. Michaela NOVAKOVA (Institute of Macromolecular Chemistry, Academy of Sciences of Czech Republic, v.v.i. Prague, Czech Republic) *Novel polymeric micelle-like structures assembled by metal ion addition designed for radiopharmaceutical purposes*	P-106	248

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	Ms. Aurélie PAPON (PPMD - ESPCI ParisTech, Paris, France) *LAOS: a new signature for the mechanics of filled elastomers*	P-108	250
	Dr. Roberto PÉREZ-APARICIO (Universidad del País Vasco - UPV/EHU, Donostia-San Sebastian, Spain) *Chain Dynamics of Poly(ethylene-alt-propylene) Melts. Bridging the Gap between Fully Atomistic and Coarse-grained Simulations*	P-109	251
	Prof. José A. POMPOSO (DIPC - Donostia International Physics Center, Donostia-San Sebastian, Spain) *Scaling law cross-over during the the collapse of polydisperse chains to unimolecular nanoparticles: Effect on SEC polysispersity*	P-110	252
	Mr. Clement RIEDEL (DIPC - Donostia International Physics Center, Donostia-San Sebastian, Spain) *Dielectric and mechanical properties of polymers at macro and nanoscale*	P-111	253
	Mr. Flavio ROMANO (Sapienza - Universitá di Roma, Roma, Italy) *Phase Diagrams of Tetrahedral Patchy Colloids: role of the interaction range and patch width*	P-112	254
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	Mr. Mohammed Zakaria SLIMANI (DIPC - Donostia International Physics Center, Donostia-San Sebastian, Spain) *Dynamic Heterogeneity in Diblock Copolymer*	P-120	262
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	Dr. Agnieszka TERCJAK (Universidad del País Vasco - UPV/EHU, Donostia-San Sebastian, Spain) *Conductive Properties of Inorganic/Organic Nanostructured Polymeric Materials Using Electrostatic and Tunneling Force Microscopy*	P-122	264
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	Ms. Grethe VESTERGAARD JENSEN (Dept. Chemistry, Interdisciplinary Nanoscience Center - iNANO, Univesity . Aarhus, Denmark) *Synchrotron SAXS Study of Micelle Formation*	P-124	266
	Dr. Ilja VOETS (Adolphe Merkle Institute, University of Fribourg, Marly, Switzerland) *Complex polymer assemblies*	P-125	267
	Dr. Lutz WILLNER (Forschungszentrum Juelich GmbH, Juelich, Germany) *Model PI-PDMS Block Copolymers - Synthesis, Characterisation and Physical Properties*	P-126	268
	Dr. Katrin WINKEL (Institute of Physical Chemistry, University of Innsbruck, Innsbruck, Austria) *Amorphous ices – the glassy states of water*	P-127	269
	Mr. Thomas ZINN (Forschungszentrum Juelich GmbH, Juelich, Germany) *Exchange kinetics in n-alkane-poly(ethylene oxide) block copolymer micelles*	P-128	270

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		Dr. Pablo ALBELLA (Centro de Física de Materiales, CSIC - UPV/EHU, Donostia-San Sebastian, Spain) *Near field study of Silicon micro-nano structures in the near infrared*	P-130	307
		Ms. Ana ASENJO GARCIA (Instituto de Óptica, CSIC, Madrid, Spain) *Dynamics of spinning particles under external illumination*	P-131	308
		Mr. Palash BHARADWAJ (University of Rochester, Rochester - MN, USA) *Plasmon-enhanced photoemission from a single rare-earth fullerene*	P-132	309
		Mr. Björn BRIAN (Chalmers University of Technology. Bionanophotonics, Applied Physics, Göteborg, Sweden) *Plasmonically Modified Resonance Energy Transfer*	P-133	310
		Mr. Daan BRINKS (ICFO - The Institute of Photonic Sciences, Castelldefels, Spain) *Coherent Control of Femtosecond Field Dynamics around Nanoantennas*	P-134	311
		Ms. Marta CASTRO-LOPEZ (ICFO - The Institute of Photonic Sciences, Castelldefels, Spain) *Polarized multiphoton emission from resonant Al, Ag and Au nanoantennas*	P-135	312
		Dr. Jianing CHEN (nanoGUNE, DIPC - Donostia International Physics Center, Donostia-San Sebastian, Spain) *Phase-Sensitive Near-field Imaging of Optical Nano-antennas*	P-136	313
		Prof. Lesley F. COHEN (Imperial College London, London, UK) *Detection of Disease Specific Enzymes Using Surface Enhanced Raman Scattering (SERS)*	P-137	314
		Prof. Lesley F. COHEN (Imperial College London, London, UK) *In-Situ Raman Spectroscopy of Graphene in Reducing Atmospheres*	P-138	315
		Ms. Christin DAVID (Instituto de Óptica, CSIC, Madrid, Spain) *Spatial Dispersion in the Optical Response of Metallic Nanoparticles using Advanced Material Models*	P-139	316

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	Dr. Ruben ESTEBAN (Centro de Física de Materiales, CSIC - UPV/EHU. DIPC - Donostia International Physics Center, Donostia-San Sebastian, Spain) *Optimizing the excitation of gap cavity modes by linear antenna modes*	P-141	318
	Mr. Aitzol GARCIA-ETXARRI (Centro de Física de Materiales, CSIC - UPV/EHU, Donostia-San Sebastian, Spain) *Engineering the Near-Field of Metallic Nanoantennas: Enhancing Possibilities in Spectroscopy and Microscopy*	P-142	319
	Dr. Vincenzo GIANNINI (Imperial College London, London, UK) *III/V Solar Cells with a Multi-Functional Plasmonic Light Concentration Layer*	P-143	320
	Dr. Raquel GÓMEZ-MEDINA (Instituto de Ciencia de Materiales de Madrid, CSIC, Madrid, Spain) *Optical interactions on small magnetodielectric particles*	P-144	321
	Mr. Nicolas GUILLOT (Université Paris 13, Bobigny, France) *Surface Enhanced Raman Scattering of gold nanostructures: Role of dipolar and multipolar localized surface plasmons*	P-145	322
	Mr. Nicolas GUILLOT (Université Paris 13, Bobigny, France) *SERS Optimization Of Gold Nanocylinders Arrays: Influence Of The Surrounding Medium And Application For Polycyclic Aromatic Hydrocarbons Detection*	P-146	323
	Mr. James T HUGALL (NanoPhotonics Centre, University of Cambridge, Cambridge, UK) *Engineered plasmonic structures: Enhanced Raman scattering and stretch tunability*	P-147	324
	Dr. Luis INCLÁN-SÁNCHEZ (Universidad Autónoma de Madrid. Departamento de Física de la Materia Condensada, Madrid, Spain) *On the Optical Conductance of Tapered Fibers*	P-148	325
	Dr. Jorge LAMELA (Universidad Autónoma de Madrid, Madrid, Spain) *Near field local enhancement by ordered arrays of sub-wavelength scattering centres fabricated by femtosecond ablation*	P-149	326
	Mr. Nicolas LARGE (CFM, CSIC - UPV/EHU. DIPC, Donostia-San Sebastian, Spain. CEMES – CNRS Université Toulose, Toulouse, France) *Acousto-plasmonic dynamics of metallic nano-objects*	P-150	327

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	Ms. Diana MARTÍN-BECERRA (IMM-Instituto de Microelectrónica de Madrid, CNM-CSIC, Tres Cantos, Spain) *Magnetic modulation of the real and imaginary part of SPP wavevector in Au/Co/Au films*	P-152	329
	Dr. Frank NEUBRECH (University Heidelberg, Heidelberg, Germany) *Symmetry forbidden infrared resonances in single metallic nanoantennas*	P-153	330
	Ms. Olalla PÉREZ-GONZÁLEZ (UPV/EHU, Leioa. DIPC - Donostia International Physics Center, Donostia-San Sebastian, Spain) *Optical spectroscopy of conductive molecular junctions in plasmonic cavities*	P-154	331
	Mr. Mohamed Ameen POYLI (DIPC - Donostia International Physics Center, Donostia-San Sebastian, Spain) *INFRARED PHONONIC NANOANTENNAS: Surface Phonon Polaritons in SiC Disks.*	P-155	332
	Mr. Rogelio RODRIGUEZ-OLIVEROS (Instituto de Estructura de la Materia, CSIC, Madrid, Spain) *Designing metal nanoantennas though bio-inspired stochastic optimization*	P-156	333
	Mr. Mikolaj SCHMIDT (Institute of Physics, Nicolaus Copernicus University, Torun, Poland) *Absorption enhancement in light-harvesting complexes coupled to plasmons in a silver island film: experiment and theory*	P-157	334
	Mr. Martin SCHNELL (nanoGUNE, Donostia-San Sebastian, Spain) *Mapping and Control of Nanoscale Optical Vector Fields*	P-158	335
	Dr. Timur SHEGAI (Chalmers Institute of Technology, Göteborg, Sweden) *Coloring fluorescence emission with silver nanowires*	P-159	336
	Prof. Clivia M. SOTOMAYOR-TORRES (Catalan Institute of Nanotechnology, ICREA, Bellaterra, Spain) *Spontaneous Emission Control of Semiconducting Nanocrystals and Dye-Molecules Embedded in Nanoimprinted Polymer Photonic Crystals via Localized Surface Plasmons*	P-160	337
	Mr. Johannes STIEGLER (nanoGUNE, Donostia-San Sebastian, Spain) *Nanoscale Free-Carrier Profiling of Individual Semiconductor Nanowires by Infrared Near-Field Plasmon Resonance Spectroscopy*	P-161	338

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	Mr. Daniel WENZLIK (Institue of Organic Chemistry, Johannes Gutenberg-University, Mainz, Germany) *Incorporation of Inorganic Nanorods into Cholesteric Liquid Crystals for Lasing Application*	P-163	340

PASSION FOR ELECTRONS

ABSTRACTS

Quantum oscillations, superconductivity, zero-bias anomalies, and Coulomb blockade in nanoscaled supported lead islands

SCHNEIDER Wolf-Dieter[1, 2]

[1]Institute of Condensed Matter Physics (ICMP), Lausanne, Switzerland
[2]Ecole Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland

Using low-temperature scanning tunneling spectroscopy down to a temperature of 3 K, we studied the linewidth of unoccupied quantum-well states in ultrathin Pb islands, grown on Si(111) on two different Pb/Si interfaces. A quantitative analysis of the differential conductance spectra allowed us to determine the electron-electron (e-e), electron-phonon (e-ph), and the interface contributions to the lifetime. Layer-dependent ab initio calculations of the e-ph linewidth contribution are in excellent agreement with the data. Importantly, the sum of the calculated e-e and e-ph lifetime broadening follows the experimentally observed quadratic energy dependence (1).

The energy gap of these superconducting Pb islands, in a thickness range between 60 and 5 monolayers, was found to decrease from its bulk value as a function of inverse island thickness. Corresponding values of the critical temperature Tc, estimated using the bulk gap-to-Tc ratio, are in quantitative agreement with ex-situ magnetic susceptibility measurements, however, in strong contrast to previous scanning probe results. Layer-dependent ab initio density functional calculations for free-standing Pb films show that the e-ph coupling constant, determining Tc, decreases with diminishing film thickness (2).

Moreover, we show that the charge transport between lead nanocontacts and various types of materials (metal, semi-metal (highly oriented pyrolitic graphite (HOPG)), semiconductor, ultrathin dielectric films on metals) varies strikingly upon reduction of the contact area, manifesting itself by the successive appearance of pseudo-gaps, Coulomb blockade and Coulomb staircases in the conductance spectra (3).

1. I.-P. Hong, C. Brun, F. Patthey, I. Yu. Sklyadneva, X. Zubizarreta, R. Heid, V. M. Silkin,
P. M. Echenique,K. P. Bohnen, E. V. Chulkov, and W.-D. Schneider,
Phys. Rev. B 80, 081409 (R) (2009).

Lifetime of optically excited electrons

AESCHLIMANN Martin[1]

[1]Dept. of Physics and Research Center OPTIMAS University of Kaiserslautern, Kaiserslautern, Germany

This talk reviews the issue of hot electron lifetimes in metals and metallic thin films, where the emphasis lies on time resolved two-photon photoemission (TR-2PPE) measurements. The dynamics of excited (hot) electrons play an important role in surface physics and chemistry. It is therefore important to address the question of how the bulk electronic structure influences the mean free path and the excited electron lifetimes. For excitation energies > 10 eV the so called universal curve allows a rather good estimate of these quantities. However, at low excitation energies ($E-E_F < 10$ eV) there are significant deviations from this approximation. In metals the relaxation process is almost exclusively attributed to the inelastic scattering with cold electrons below the Fermi level (e-e scattering) and with phonons (e-ph scattering).

Using the time resolved two-photon photoelectron spectroscopy (TR-2PPE) method we investigated the electron dynamics in aluminium, various noble, transition and rare earth metals up to excitation energies of $E-E_F = 4.5$ eV. The characteristics of the electronic structure of the respective metal classes responsible for energy dissipation processes of hot electrons will be analyzed.

In the second part TR-2PPE studies on the two-dimensional metallic quantum well systems Pb/Cu(111) and Bi/Cu(111) will be reported. Our investigations focus not only on the energetic dependence, but also on the momentum dependence of the hot electron dynamics, i.e., the relevance of band-structure details $E(k_{||})$ to the decay of hot electrons. Quantum-well systems are well suited for these investigations since they exhibit interesting characteristics in their electronic band-structure, which potentially can affect the excited state lifetime in specific areas in momentum space. This includes, e.g., avoided crossings of bands or k-localized band gaps.

As an outlook, the hot electron lifetimes in organic semiconductors will be discussed.

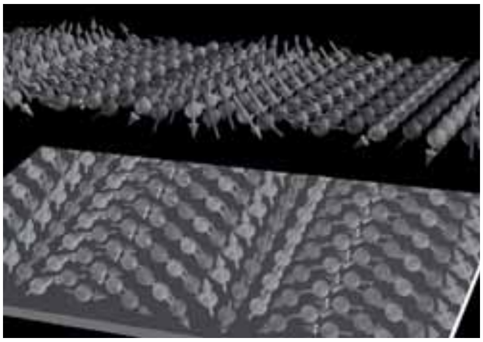
Invited Lectures / Oral Contributions | 11:40 | 30 SEPT.

Electrons at surfaces: From Rashba effect to topologically protected spin textures

BLÜGEL Stefan[1]

[1]Institut für Festkörperforschung and for Advanced Simulation Forschungszentrum Juelich and JARA, Juelich, Germany

The surface and interface is distinguished from ordinary bulk physics by the presence of spin-orbit interaction in a structure inversion asymmetric environment that gives rise to the well-known Rashba effect [1,2], but also to unexpected and largely unexplored phenomena such as topological insulators. I discuss the Rashba effect at surfaces of Bi and Bi-alloys and discuss then consequences for the spin-dependent scattering and the magnetic interaction. I focus at the Dzyaloshinskii-Moriya interaction caused by spin-polarized electrons in the structure inversion asymmetric environment of 3d metal films on W substrates. We found that due to the large spin-orbit interaction of the W substrate the Dzyaloshinskii interaction exceeds a critical strength and competes with the exchange interaction and causes the formation of one-dimensional cycloidal magnetic spirals of unique winding sense [3,4]. Also the effect of the Dzyaloshinskii-Moriya interaction on the domain-walls [5] or the exchange bias will be discussed. Going one step further we raise the questions can we design surfaces that do not exhibit a lattice of one-dimensional but two-dimensional non-trivial magnetic structures, known as Skyrmions.



Homochiral magnetic order in a one-atomic layer thick film of Mn atoms on a W(110) surface. The local magnetic moments at Mn atoms shown as red and green arrows are aligned anti-ferromag-netically between nearest-neighbor atoms. Superimposed is a spiral pattern of unirotational direction. The top picture shows a left-rotating cycloidal spiral, which was found in nature. The bottom picture shows the mirror image, a right rotating spiral that does not exist in nature [3].

Acknowledgement:
This work was done in collaboration with Marcus Heide, Samir Lounis, Gustav Bihlmayer, Stefan Heinze from the theory side and Matthias Bode, Andre Kubetzka, Kirsten von Berg-mann of the Wiesendanger group from the experimental side.

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Decay mechanisms of electron excitations on clean and nanostructured metal surfaces

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Interaction between lattice and electron subsystems as well as interaction within each of these subsystems is crucial to understand mechanisms of single-particle excitation dynamics, i.e. lifetime of excitations. The lifetime sets the duration of excitation and in combination with the velocity determines the mean free path, a measure of influence of the excitation.

In this presentation recent theoretical results on the decay of excited electrons and holes on clean metal surfaces, at single adatoms, at islands as well as in overlayers and free standing thin films are discussed. Different decay mechanisms and different kinds of interactions - elastic and inelastic electron-electron (e-e) interaction as well as electron-phonon (e-ph) interaction and the role of spin (spin-orbit and exchange interaction) - are analysed. E-ph decay channel is shown to be important for all systems considered. In the e-e decay channel the electron (hole) decay can be realized via creation of electron-hole pairs or plasmon excitation. Dimensionality effects in the lifetime of electrons and holes on metal surfaces and the role of screening and intra- (inter-) band transitions are also discussed.

Magnetic transitions induced by tunnelling electrons in individual adsorbates

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Recently, several IETS (Inelastic Electron Tunneling Spectroscopy) experiments[1-4] demonstrated the existence of magnetic anisotropy in individual adsorbates, i.e. different energy levels of an adsorbate exist that can be associated to different orientations of the adsorbate spin with respect to its surroundings. They also revealed that tunnelling electrons were extremely efficient in inducing transitions among these magnetic states.

We developed a strong coupling approach of the magnetic transitions induced by electrons tunnelling through an individual adsorbate[5-6]. It joins a DFT-description of the system with a sudden approximation of the magnetic excitation process. It has been successfully applied to several systems, which will be presented at the conference: Mn and Fe atoms on CuN/Cu(100) surface, Fe-Phthalocyanine molecules on CuO/Cu(110) surfaces. Besides providing a quantitative account of the inelastic process, our approach also provides a physical picture of the spin transitions during tunnelling: it appears as the direct consequence of a coupling/decoupling sequence between the spin of the tunnelling electron and that of the adsorbate. It thus directly explains the possibility of extremely large probabilities for magnetic transitions; the inelastic contributions to the tunnelling current are easily overcoming the elastic contribution. This makes the magnetic transitions very much different from other inelastic processes induced by tunnelling electrons such as vibrational excitation. The same view can also be applied to the problem of the de-excitation of magnetic states: the interaction between the substrate electrons and an adsorbate can efficiently quench a magnetic excitation via electron-hole pair creations in a way similar to the magnetic excitation induced by tunnelling electrons.

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Ultrafast electron dynamics in pump-probe spectroscopies of surfaces: from transient excitonic to quasi-stationary polaronic states

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Rapid development of pump-probe spectroscopies has greatly advanced the studies of electronic excitations in the real time domain. State- and time- resolved two-photon-photoemission (TR2PPE) measurements utilizing ultrashort laser pulses with variable delay have provided unprecendented insight into the dynamics of quasiparticles at metal surfaces. This has enabled detailed investigations of quasi–particle energetics and decay in the intermediate states of 2PPE from quasi-two–dimensional surface bands which are of fundamental interest in many aspects of surface science. In particular, occupied surface state-(SS) and unoccupied image potential-state (IS) bands constitute ideal prototype systems for studying ultrafast quasiparticle dynamics and relaxation phenomena in restricted dimensionality. So far the majority of analyses of 2PPE data from surface bands have invoked pre–existent SS-and IS-states whose many-body properties were assessed *a posteriori* by perturbation methods. However, since IS-bands arise from an interplay of the surface band gap and retarded polarization interaction, the image potential sup–ported IS-states are fully developed only after the completion of screening of excited quasiparticle charges on the time scale of several surface plasmon cycles. Consequently, such states are mainly inaccessible in ultrafast measurements utilizing laser pulses of few femtosecond duration and delay. Instead, the evolution of an optically excited electron with energy below the vacuum level and a SS-band hole in the intermediate state of TR2PPE should be visualized as a transient exciton which with the formation of image charge evolves into a weakly correlated quasi–particle pair (IS-electron+SS-hole). The corresponding many-body scenario maps onto the problem of propagation of an electron-hole pair initially governed by ex–citonic interactions which in the course of time give way to polaronic interactions of each quasiparticle with the developing screening cloud and thereby to establish–ment of IS-band states. Temporal stages of these processes will be illustrated and quantied on the paradigmatic example of 2PPE from Cu(111) surfaces.

Coherent dynamics of image-potential electrons

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The Rydberg series of images-potential states represent an attractive model system for exploring coherent electron dynamics at metal surfaces. Well-known examples are quantum-beat spectroscopy and wave-packet excitation of states with high quantum numbers, phase-dependent photoemission, and the generation of coherently controlled currents at metal surfaces. Whereas these previous experiments benefited from a relatively weak interaction of the states with the bulk metal, several intriguing effects are expected to occur in the other limit, when image-potential resonances are strongly coupled to a continuum of states in the volume. Model calculations show that interference effects can lead to unexpected peak narrowing, peak shifting and even to peak suppression or the trapping of electronic excitations. I will report about two-photon-photoemission (2PPE) experiments for Al(100) surfaces where some of these effects are expected to be present. Al(100) has only a small gap in the projected bulk bands at the Γ-point and the image-potential resonances are located more than 5 eV above this gap. This results in a very strong coupling of the resonances with the unoccupied bulk states. We observe that the n=1 resonance is almost completely suppressed by destructive interference whereas the resonances n=2,3,4,5 are clearly resolved in the time-resolved spectra and have lifetimes up to 140 fs.

29 SEPT. | 12:20 | Invited Lectures / Oral Contributions

The electronic structure of graphene: confinement-induced band gap opening and core electron delocalization

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Graphene, a two-dimensional layer of carbon atoms, has received enormous attention since its isolation a few years ago, both as a playing ground for fundamental physics and a a promising material for future semiconductor applications. This talk is concerned with two aspects of graphene´s electronic structure which touch upon both themes.

On the fundamental side, we show that the carbon 1s electrons in graphene show band-like dispersion, despite of their high binding energy of 284 eV. The dispersion is described by the simple formation of a bonding and an anti-bonding band between the two atoms in the unit cell of graphene. Due to a Young´s double slit-like interference effect, a situation arises in which only the bonding or only the anti-bonding state is observed for a given photoemission geometry. Bonding / anti-bonding splitting of deep core levels has been observed in small and strongly bound molecules, such a nitrogen or acetylene, but graphene is the first solid in which this has been found.

On the more applied side, we report the observation of a band gap formation in the valence band of graphene. Graphene is a semimetal with a vanishing density of states at the Fermi level but no band gap. While the electronic properties are otherwise extremely promising for semiconductor applications (high mobility, linear dispersion), the absence of a band gap is a serious obstacle. Combining angle-resolved photoemission spectroscopy and scanning tunneling microscopy, we show that a significant band gap can be introduced in supported graphene layers by a quantum confinement effect through patterned adsorption of hydrogen.

Attosecond spectroscopy on solid surfaces

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Atoms exposed to a few oscillation cycles of intense visible or near-infrared light are able to emit a single electron and XUV photon wavepacket of sub-femtosecond duration [1,2]. Precise control of these sub-femtosecond wavepackets have been achieved by full control of the electromagnetic field in few-cycle light pulses [3]. These XUV pulses together with the few-cycle (few-femtosecond) laser pulses used for their generation have opened the way to the development of a technique for attosecond sampling of electrons ejected from atoms [4], molecules, and solids. This is accomplished by probing electron emission with the oscillating electric field of the few-cycle laser pulse following excitation of the atom by the synchronized sub-femtosecond XUV pulse. Sampling the emission of photo electrons in this manner allows time-resolved measurement of the XUV pulse duration as well as of the laser field oscillations [5].

After the full characterization of these tools, first experiments have been carried out to measure sub-femtosecond behavior of matter. Recently, the dynamics of the photoionization process on solids has been studied [6]. Not only that attosecond metrology now enables clocking on surface dynamics, but also the individual behaviour of electrons of different type (core electrons vs. conduction band electrons) can be resolved. We measured a time delay of about 100 as on the emission of the aforemention two types of electrons in different solid probes. We investigate electron transport in different materials with adlayers of varing thickness to gain information on transport effects and other material properties. The information gained in these experiments may have influence on the development of many modern technologies including semiconductor and molecular electronics, optoelectronics, information processing, photovoltaics, electrochemical reactions, electronically stimulated chemistry on surfaces and interfaces, non-adiabatic reactions, optical nano-structuring, and interference effects in spectroscopy.

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28 SEPT. | 15:00 | Invited Lectures / Oral Contributions

Experiments on the exchange-correlation hole in solids

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The concept of the exchange-correlation hole (xc-hole) is fundamental to solid state physics. It was introduced in the early 1930ies by Wigner and Seitz and Slater, and postulates, that each electron in a solid is surrounded by a region of reduced electronic charge, adding up to exactly one electron charge. Thus, each such “dressed” electron looks “neutral” to another one residing beyond a certain distance. This concept explained why electrons essentially behave like independent quasi-particles. Despite the success of this postulate it has never been directly tested experimentally for the past 70 years. In order to do this, one has to make a scattering experiment, which by the very nature of the dressed electrons must have a rather small cross section.

We set up an (e,2e) experiment in which an electron (of some 10 eV kinetic energy) is sent to a sample, is elastically back reflected and on its way out may scatter with a valence electron. There are cases where the incident and the hit electron may have sufficient energy to overcome the surface barrier and may be detected in vacuum. (needless to say that they are indistinguishable). For a given emission direction of the one electron the electron-electron interaction manifests itself in the angular distribution of the second electron around this direction. We made such experiments and found that there is a depletion zone for the second electron within an angular range of about 1 rad, essentially independent of its energy. We tested this for alkali halides as well as for Cu with somewhat different results. Since the cause of this effect is the same as the reason for the xc-hole, namely the mutual repulsion of electrons by exchange interaction and Coulomb repulsion, one may eventually map experimentally the xc-hole. In order to disentangle the contributions from correlation and exchange, one may work with a spin-polarized target and spin-polarized primary electrons. Such an experiment has been carried out recently /1/, using Fe as the target and a GaAs photocathode electron source. We find that the “exchange hole” is significantly larger than the “correlation hole”. Another approach might be to use positrons as primary particles. Since positrons and electrons are distinguishable, the exchange interaction would be turned off. A first proof-of-principle-experiment /2/ shows that a (p, ep) experiment is possible, despite the competing positron-electron annihilation process.

*in collaboration with F. Schumann, and C. Winkler

/1/ Spin-resolved mapping of spin contribution to exchange-correlation holes
F. O. Schumann, C. Winkler, J. Kirschner, F. Giebels, H. Gollisch, and R. Feder
Phys. Rev. Lett. 104, 087602 (2010)
/2/ Correlated positron-electron emission from surfaces
G. van Riessen, F. O. Schumann, M. Birke, C. Winkler, and J. Kirschner
J. Phys.: Cond. Matt. 20, 442001 (2008)

Electron Localization following Attosecond Molecular Photoionization of H_2

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The development of attosecond laser pulses allows one to probe the inner workings of atoms and molecules on the timescale of the electronic response. In molecules, attosecond pump-probe spectroscopy enables investigations of the prompt charge redistribution and localization that accompany photo-excitation processes, where a molecule is lifted from the ground Born-Oppenheimer potential energy surface to one or more excited surfaces, and where subsequent photochemistry evolves on femtosecond timescales. Here we present the first example of a realistic molecular attosecond pump-probe theoretical calculation. H2 and D2 are dissociatively ionized by the sequence of an isolated attosecond pulse and an intense infrared few-cycle pulse. A localization of the electronic charge distribution within the molecule is calculated that depends – with attosecond time-resolution – on the delay between the pump and probe pulses. The results of these calculations are compared with recent experimental measurements and allow us to propose two different mechanisms that explain the observations.

28 SEPT. | 10:35 | Invited Lectures / Oral Contributions

Plasmon propagation and confinement in atom-scale chains and sheets

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Size effects and shape effects strongly affect the electronic excitations in nanomater-scale metallic objects and hence determine the optical properties of the nanomaterials. We show some examples of the plasmonic ex-citations in atomically thin metal films and wires. The two-dimensional type plasmon is observed in metallic atom sheets and the one-dimensional type plasmons are also measured from some metallic atom chains.

When the size of the object shrinks beyond micrometer scale and it reaches down to nanometer or sub-nanometer scale, novel effects that originate from its smallness come into view. The most common and import-ant effect is the size effect, or the confinement effect. Plasmons in metallic tiny objects show pronounced size/shape effects in reduced dimensions, especially in nanometer scale. This fits perfectly to the demand for developing the new functional properties at the nanoscale/atomscale for the next generation nano-photonics/optics device materials. In this context, not only from the scientific point of view but also from the technical point of view, it is of great importance to clarify whether plasmons are confined and can propagate in atom-scale small objects such as in atom chains atom sheet etc. This kind of investigation will be the first step towards the realization of the ultimately small atom-scale/nano-scale optics. In the present talk, I will introduce our recent works on these shape effects, dimensionality effects, Rashba effects, as well as antenna resonance found in atom-scale plasmons.

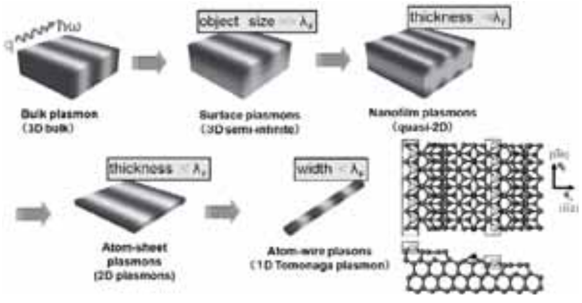

Fig. 1: Schematics of the charge density oscillations of the plasmons in various dimensions.

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Imaging the femtosecond time scale correlated electron-nuclear dynamics in surface photodesorption

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We employ time-resolved two-photon photoemission to characterize electronic structure and photoinduced dynamics of chemisorbed alkali atoms on noble metal surfaces. Photoinduced charge transfer excitation of the lowest energy sigma resonance of Cs on Cu or Ag surfaces turns on repulsive forces between atom and surface initiating nuclear wave packet motion on a dissociative potential energy surface. Energy, momentum, and time resolved measurements of photoemission from desorbing atoms provide information on the nuclear wave packet motion and the concomitant changes in the surface electronic structure. In particular, we use time-dependent momentum imaging of photoemission from the excited state to explore the correlation between the electron and nuclear motions.

30 SEPT. | 09:50 | Invited Lectures / Oral Contributions

The asymptotic behavior of the Kohn-Sham potential of Density-Functional Theory at metal surfaces

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A long-standing puzzle in density-functional theory is the issue of the long-range behavior of the Kohn-Sham (KS) exchange-correlation (xc) potential at metal surfaces. As an important step toward its solution, it is proven here, through a rigorous asymptotic analysis and an accurate numerical solution of the optimized-effective-potential integral equation, that the KS exact-exchange potential decays as ln(z)/z far into the vacuum-size of an extended metal surface. On the other hand, it is suggested here that the long-range behavior of the full KS xc potential at metal surfaces should be expected to be dominated by the surface-plasmon field responsible for the creation of a flat xc hole located at the so-called image plane.

Acoustic Surface Plasmons, a novel collective excitation at metal surfaces, with promising applications

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The Acoustic Surface Plasmon (ASP) are a novel collective electronic excitation, arising from the 2-dim electron gas of the Shockley surface state (SSS) at metal surfaces. It was forecasted for all metal surfaces and reported recently for Be [1], Cu [2] and Au [3] surfaces and opening up a new and promising field of research and applications.

Contrary to ordinary Surface Plasmons, characterised by a finite frequency also in the limit of large wavelengths, the ASP exists at all energies and can thus play a role in the energy dissipation processes determining e.g. the outcome of gas-surface interaction processes and of catalytic chemical reactions in the heterogeneous phase.

Even more important, given the linear dependence of the ASP frequency on inverse wavelength, an ASP based plasmonic signal can propagate over the surface without distortion. Novel ASP based opto-plasmonic devices transforming light into plasmon signals, similar to existing photonic devices, can thus be envisaged. Since the wavelength of an excitation at a given frequency is determined by its propagation velocity, ASPs are about 1000 times smaller than the corresponding photons. A future ASP based device could thus be up to 1000 times smaller than a photonic one.

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First principle modeling of the excited state properties of complex nanostructures and biomolecules: a TDDFT and Many-Body perturbation theory approach

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There has been much progress in the synthesis and characterization of nanostructures however, there remain immense challenges in understanding their properties and interactions with external probes in order to realize their tremendous potential for applications (molecular electronics, nanoscale opto-electronic devices, light harvesting and emitting nanostructures). In this talk we will review the recent advances within density-functional based schemes to describe spectroscopic properties of those complex systems. Special emphasis will be made in modeling new materials and simulate new time and spatially resolved spectroscopies. We will address both linear and non-linear response regimes to study the optical absorption of biological chromophores, one-dimensional polymers and layered materials. Moreover, we will illustrate how an optimal control theory can be implemented such that we could have control of the quantum state of a molecular structure (for example addressing qbits in 2D nanostructures, high harmonic generation, etc).

Within the goal of spanning larger time-scales and more complex structures, we will describe a new method to mimic the electron-ion dynamics within the Ehrenfest scheme where no explicit orthogonalization is necessary and we can increase of the time step while keeping the system close to the Born-Oppenheimer surface. The method is easily implemented and scales very well with the system size. Applications to the excited state dynamics in some organic molecules will be used as text cases to illustrate the performance of the approach. In particular we will show the effect of electron-hole attraction in those systems. Pros and cons of present functionals will be highlighted and provide insight in how to overcome those limitations by merging concepts from many-body perturbation theory and time-dependent density functional theory.

All those developments constitute a basic ingredient for the realization of the European Theoretical Spectroscopy Facility (ETSF, http://etsf.eu) as a top-level scientific infrastructure.

Invited Lectures / Oral Contributions | 12:50 | 29 SEPT. |

Ultrafast demagnetization dynamics in ferromagnets and Heusler alloys

SCHNEIDER Hans Christian[1], STEIL Daniel[1], ALEBRAND Sabine[1], KRAUSS Michael[1], ROTH Tobias[1], ESSERT Sven[1], CINCHETTI Mirko[1], AESCHLIMANN Martin[1]

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We present recent theoretical and experimental results for the ultrafast magnetization dynamics of ferromagnets and Heusler alloys, the latter exhibiting a band gap in one spin channel.

We compare time-resolved magneto-optical Kerr effect (TR-MOKE) measurements with dynamical calculations based on the Elliott(-Yafet) spin-relaxation mechanism [1], which include the spin-orbit interaction in the band structure and the spin-diagonal Coulomb scattering at the level of momentum-resolved Boltzmann scattering integrals.

For cobalt and nickel we find good agreement with experiment by fitting the fluence and the spin-orbit interaction strength. We explain the difference in the maximum magnetization quenching between cobalt and nickel by the dependence of the magnetization dynamics on available optical and scattering transitions.

Band structure calculations indicate that the Heusler alloys CMS and CFS investigated by us differ in the lineup of the gap in the minority-spin channel. Only for CMS [2] the gap is above the Fermi energy in the minority channel, which leads to a lack of empty minority-electron states above the Fermi energy. This electronic "minority-state blocking" should prevent spin flips from optically excited majority electrons and thus slow down the demgnetization dynamics. However, in the experiment, there is no pronounced difference between the magnetization dynamics of CMS and that of the similar compound CFS, which do*es* not show electronic minority-state blocking. Calculations show that the fast demagnetization in CMS may take place via spin-flip transitions below the Fermi energy where the final states have been depopulated by the optical excitation.

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Interface states in carbon nanotube junctions: rolling up graphene

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We study the origin of interface states in carbon nanotube intramolecular junctions between achiral tubes. By applying the Born-von Karman boundary condition to an interface between armchair- and zigzag-terminated graphene layers, we are able to explain their number and energies. We show that these interface states, costumarily attributed to the presence of topological defects, are actually related to zigzag-edge states, as those of graphene zigzag nanoribbons. Spatial localization of interface states is seen to vary greatly and may extend appreciably into either side of the junction. Our results give an alternative explanation to the unusual decay length measured for interface states of semiconductor nanotube junctions and could be further tested by local probe spectroscopies.

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Exchange interaction between localized spins in non-equilibrium

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The electron mediated exchange interaction between local spins adsorbed on two-dimensional surface is studied under non-equilibrium conditions. The effective spin-spin interaction is found to depend both on time and the spin-polarization of the substrate and the excitation spectrum of the local spins. For spatially anisotropic spin-polarization of the substrate, the spatial dependence of the interaction comprise components decaying as $\sin(2k_FR)/(2k_FR)$ and $\sin(2k_FR)/(2k_FR)^2$.

0-03

Laser pulse length dependence of electron and nuclear dynamics in Coulomb explosions of xenon clusters

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This contribution reports on trajectory calculations of Xe_n clusters (n=55-6099) irradiated by ultraintense laser pulses (peak intensities $I_M = 10^{15}$-10^{17} Wcm ^{2}, pulse lengths t = 25-230 fs, frequency 0.35 fs^{-1}). The simulations showed that for long pulses (t = 230 fs), even at low laser intensity (10^{15} Wcm^{-2}), the nanoplasma electrons assume high average kinetic energies (»700 eV), enhancing both impact ionization and outer ionization drastically. Thereby, the maximum electron kinetic energies occur after rather than at the peak of the laser pulse, indicating that the nanoplasma possibly passes a resonance with the laser field. The enhanced depletion of the nanoplasma electrons by outer ionization leads to much higher final ion kinetic energies and to a qualitatively different cluster size dependence of ion kinetic energies than for short pulses. The situation is completely different for short pulses (t = 25 fs), where average electron kinetic energies are much smaller, inner ionization is dominated by field ionization and outer ionization occurs at a much lower level.

Invited Lectures / Oral Contributions | 10:50 | 30 SEPT.

Some aspects of the theory of streaking experiments with sub-femtosecond pulses on solids.

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The sub-femtosecond XUV pulse technique initiated by [1] has its aim to study super-fast relaxation processes caused by an abrupt change in the electron subsystem after an electron ejection. Up to now the main method of observation of the processes induced by the XUV pulse absorption is the so-called streaking method which allows to transform the development of the processes in the time-domain into the energy spectra of the ejected electrons [2]. This is not a direct observation method and therefore development of an adequate theory is of paramount importance

Application of sub-femtosecond technique to solids is of great interest because a vast number of transient electron phenomena at surfaces and in bulk does evolve on a few femtosecond – sub-femtosecond time scale. Although the dynamics of electrons in condensed matter is very complicated, its comprehensive theoretical understanding is necessary for promoting experimental investigations and their applications in nanotechnology. Currently only one experiment with the sub-femtosecond technique applied to solid state system has been performed [3]. The corresponding theory was presented in [4] and its physical content will be briefly presented in the talk. Our explanation of the experimental finding is based on the fact that the mean-free path of electrons in a metal is very short while a low-frequency IR field is promptly screened in a metal.

The principle objects of study with the sub-femtosecond technique are various relaxation processes. One of such processes, dynamical screening of the field of an electron receding from a solid surface, will be discussed. Also, it is planned to discuss the possibility of observation of a hole screening in solids with strudy of streaking of electrons ejected due to the Auger processes in embedded atoms.

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28 SEPT. | 15:30 | Invited Lectures / Oral Contributions

Modeling XUV-NIR streaking experiments at metal surfaces

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Over the past few years the interest in streaking experiments has shifted to multi-electron systems among them even metals. Run-time differences for electrons released at different energies were observed in some cases exceeding the expected delay by a factor of 2 or larger.

We have developed a model for streaking at metal surfaces based on a classical transport theory for electrons photo-excited by the XUV pulse and propagated in the field of the probing ultrashort NIR pulse.

We are able to reproduce energy and streaking spectra of emitted electrons for systems ranging from (almost) free electron gas metals (Al, Mg) to transition materials with a more complicated electronic structure (W). While in the latter case various contributions to the energy spectrum renders the deconvolution of timing information contained in the streaking spectrum almost impossible Al and Mg show well separated lines with a simple interpretation which might allow for a discrimination of different models for the dispersion relation of electrons in metals irradiated by intense ultrashort laser pulses.

Plasmon tsunami on C_{60} caused by electron transfer to a highly charged ion

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An electron violently stripped away from a fullerene molecule by a flying-by, highly charged ion leaves behind a plasmon quantum tsunami. A quantum tsunami consists of a coherent state of collective excitations. The charge transfer confers an energy gain to the ion minus the energy required to excite the plasmon coherent states: a new tool to investigate energetic collective excitations in nanostructures.

NO photochemistry on silver nanoparticles by nanosecond vs. femtosecond excitation

MENZEL Dietrich[1, 2], KIM Ki Hyun[1], MULUGETA Daniel[1], WATANABE Kazuo[3], FREUND Hajo[1]

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The special electronic and optical properties of metal nanoparticles (MNPs), notably plasmon excitation and confinement of excitations, lead to drastic changes of surface photochemistry [1]. We have previously demonstrated strong influences of the initial excitation, and of the mean particle size, on the photodesorption cross sections (PCS) of NO from NO dimer layers on oxide-supported AgNPs [2,3], using nanosecond laser pulses. The mechanism, however, remains the same as on Ag(111) over most of the range, as indicated by measurements of final state energy distributions on the desorbing molecules [4]; it is believed to go via transient negative ions [5]. Strictly linear behavior is found. Recent femtosecond measurements, however, show strong nonlinearity and changes of PCS and energy distributions for small particles indicating a new mechanism, while the mechanism of desorption remains the same for Ag(111). We will discuss the interpretation of the previous and the new results, aiming at conclusions about their relevance for the understanding of nanoparticle excitations and photochemistry.

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Performance of the exchange-correlation kernel of time-dependent density-functional theory derived from LDA to current-density functional theory

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The scalar and tensor exchange-correlation kernels (f_{xc}) are the key quantities in the time-dependent density functional theory and the time-dependent current density functional theory, respectively. It is known that the local-density approximation (LDA) is both inaccurate and intrinsically inconsistent to be used in construction of the scalar f_{xc}. On the other hand, the tensor f_{xc} is amenable to LDA treatment, although the accuracy depends on the specific system and the range of the frequency. Exact [1] (a rather complicated) and approximate [2] (easy-to-use, recently derived) formulas exist which express the scalar f_{xc} via its tensor counterpart. Scalar f_xc obtained through these formulas by the substitution of the LDA to the tensor f_xc is not LDA to the scalar f_xc, but this rather is a promising non-local approximation possessing some properties the exact scalar f_{xc} must have: It satisfies the zero-force sum-rule for finite systems and has the 1/q^2 singularity in the periodic case. We present results of calculations of optical spectra of semiconductors obtained within this approach. A tendency to the correction of the Kohn-Sham band gaps and the overall shift of the spectra to better agreement with experiment compared to TDLDA is observed and the refinements of the method are discussed.

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30 SEPT. | 13:10 | Invited Lectures / Oral Contributions

Ultrafast dynamics of coherent phonons during the insulator-metal transition of VO_2

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VO_2 exhibits a first-order phase transition (PT) from an insulating, monoclinic to a metallic, rutile phase at 67 °C. Though studied in detail in the past decades by a large number of experimental and theoretical approaches, uncertainty remains about whether lattice deformation (Peirls) or strong electron correlation (Mott) dominate the transition. Femto- and picosecond time-resolved studies of the *photoinduced* transition are a promising tool to achieve better understanding of the underlying processes, as they may provide temporal separation of the lattice and charge carrier dynamics of the PT.

In the present work, we investigate the ultrafast response of a 200 nm thin VO_2 film to optical excitation (pump) in a wide range of fluences up to 30 mJ/cm^2. The resulting non-equilibrium ultrafast dynamics are probed by means of optical spectroscopy (800 nm, < 40 fs). At low excitation densities, the transient reflectivity response of hot carriers, which decays with a time constant of 400 fs, is superimposed with four coherent phonon modes of monoclinic VO_2 that are observed up to several ps. These modes, however, persist even when the pump fluence is increased above 10 mJ/cm^2, an excitation density that is commonly assumed to drive the transition to the rutile metallic phase. Only at even larger fluences (> 20 mJ/cm^2), these coherent phonons, which are characteristic for the *monoclinic* VO2 structure, are ultimately suppressed, indicating completion of the structural transition. Providing insight into the lattice dynamics during the insulator-metal transition of VO_2, these results will be related to previous time-resolved studies and discussed regarding potential disentanglement of Mott and Peirls contributions to the PT.

The Electronic Structure Graphane and Graphane Nanostructures from Ab Initio Theory

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Using density functional theory (DFT) we have investigated the electronic structure of the intrinsic two-dimensional (2D) graphane and substituted graphanes. We found the conduction band of graphane has nearly free electron properties, which are derived from both the image potential and the attractive potential of H atoms. We dubbed this state the 'Wet image state', because it resembles both the image potential states of a molecular sheet[1,2] and the wet electron states of dangling H atoms at solid/vacuum interfaces.[3] The electronic structure of fluorine-substituted graphane is very sensitive to the doping configuration, and its band gap can be tuned by different doping functionalization. By wrapping the 2D F-doped graphane into 1D nanotube, the 2D wet image states convert into 1D wet image states, which is NFE like and completely confined in the F-doped graphane nanotube. The diffuse character of image potential states, wet electron states and the wet image states provide electron transfer path way through space rather than through the chemical bonds. This type of conduction is potentially interesting for design of new molecular electronic materials with novel electronic properties.

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Single adatoms on 1D modulated potential: an embedding approach

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The interaction between localized atomic electrons and the conduction ones in the continuous band of a metal substrate is at the basis of a large variety of physical processes. We have developed an ab initio embedding method to treat the adsorption of a single atom on an extended substrate described by a 1D modulated pseudo-potential. The obtained results show that, accounting for the relevant electronic properties of the substrate (surface states, surface projected energy gaps), the characterization of the atomic resonances (binding energy, elastic lifetime, etc.) results improved with respect to a jellium surface.

Electron-Electron and Electron-Hole Bi-Layers in Ultra-Thin Silicon Channels

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Electron-electron and electron-hole bi-layers provide interesting systems for investigation of interactions between two carrier distributions. One example is the drag resistance between the two carrier systems. Silicon-on-insulator substrates allow fabrication of double gate devices in which the carrier density, distribution and location can be tuned inside the channel. This facilitates, for example, volume inversion/accumulation in the channel and, consequently mobility enhancement at room temperature [1], or resonance effects at low temperatures [2]. The dielectric strength of silicon dioxide makes it possible to have simultaneously electron and hole gases at the opposite interfaces of a 20 nm thick Si quantum well by highly asymmetric gate fields, as demonstrated for the first time in 2008 [3]. The drag resistance between electrons and holes is of the order of a few hundred ohms at room temperature. At temperatures below 100 K the electron-hole bi-layer show activated bi-stable behaviour. In this presentation we will show results obtained from electron-electron and electron-hole bi-layers at low and room temperature.

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29 SEPT. | 15:00 | Poster Session

Is the surface of Pd(110) magnetic?

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Investigating materials with low dimensional properties often surprises with unconventional behaviour as such systems exhibit a puzzling variety of phases.

A low-dimensional Tamm-type surface resonance is found at S-bar for both, the clean Pd(110) surface as well as for the isoelectronic Pt(110) system. The energetic position of this state is found to be atypically independent of hydrogen coverage on Pt(110) and is slightly below the Fermi-energy (EF) [1]. Hydrogen adsorption on Pd(110) takes place on different adsorption sites. Thus the surface resonance shifts from slightly above EF to below with increasing exposure, which is in accordance with theory [2]. Interestingly, upon hydrogen adsorption the pairing-row reconstruction on Pd(110) develops together with a satellite peak of the S-bar resonance. The energy distribution curves are strikingly similar to those of clean Ni(110) [3]. The band dispersion of this satellite is parallel to the dispersion of the main resonance, but shifted to lower energies by roughly 350meV.

The appearance of this satellite peak results presumably from an increased electronic correlation in the pairing-row reconstructed surface. Bulk Pd has a large density of states at the Fermi-energy which contributes to a large exchange enhanced susceptibility, revealing bulk Pd to be nearly ferromagnetic. Thus it is not surprising that theoretical investigations predict magnetic moments of ~0.7μB for monatomic wires due to the 4d band-narrowing and its low dimensionality [4]. The pairing row reconstructed surface, with its reduced coordination number, seems to be a good candidate for the observation of a paramagnetic-ferromagnetic transition. Surface-states or resonances are very sensitive to the local magnetic order at the surface and act as a surface localized magnetometer. DFT calculations including spin polarization are in progress.

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Poster Session | 15:00 | 29 SEPT.

Interface States in Carbon Nanotube Junctions: Rolling up graphene

AYUELA Andrés[1], SANTOS Hernán[2], JASKÓLSKI Wladimiersz[3], PELC Marta[3], CHICO Leonor[4]

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The presence of interface states in the CNT junctions is critical to the electronic transport and photelectron spectroscopy measurements. We study the origin of interface states in carbon nanotube intramolecular junctions between achiral tubes. We have found that the number of these states increases with diameter, following a multiple-of-three rule.

By applying the Born-von Karman boundary condition to an interface between armchair- and zigzag-terminated graphene layers, we are able to obtain their number and energy.

Ab initio calculations of zigzag/armchair superlattices provide insight into the changes due to electron-electron interactions, and elucidates the validity of the simpler tight-binding approach.

- Santos H, Ayuela A, Jaskolski W, et al. Phys. Rev. B 80, 035436 (2009)
- Ayuela A, Jaskolski W, Pelc M, et al. App. Phys. Lett 93, 133106 (2008)
- Ayuela A, Chico L, Jaskolski W Phys Rev B 77, 085435 (2008)

29 SEPT. | 15:00 | Poster Session

Interface States in Carbon Nanotube Junctions: Rolling up graphene

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- Ayuela A, Chico L, Jaskolski W Phys Rev B 77, 085435 (2008)

LT-STS study of atomic nanowires on Cu_3N/Cu(110) surface

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Self-organized growth of surface supported nano-structures like atomic nanowires are likely to play an important role in future electronic devices where the confined electrons show quantization phenomena. The formation and growth behavior of epitaxial atomic nanowires of *3d, 4d* and *5d* elements on a corrugated molecular Cu_3N network on a Cu(110) surface have been reported. An element independent growth of nanowires consisting of 5 atomic rows (~ 1 nm in width) running along [1-10] direction on Cu_3N-Cu(110) surface was observed [1]. The charge density of Cu(110) surface can be dramatically altered by terminating the Cu(110) surfaces with a (2x3) copper nitride (Cu_3N) layer. A proper understanding of the electronic structure of the Cu_3N-Cu(110) surface and the atomic nanowires grown on this surface would be fundamentally important. We report here the low temperature (~ 5 K) scanning tunneling spectroscopy (LT-STS) studies of both the Cu_3N layer and the Fe, Au and Cu atomic nanowires grown at room temperature on this surface. Both constant height and constant current spectroscopy measurements have been performed to understand the electronic structure of Cu_3N surface and of the atomic nanowires. Constant height LT-STS studies on the Cu_3N surface show that the surface is semiconducting with a band gap of around 2 eV without any pronounced electronic state appearing in the spectra. However, the constant current spectroscopy measurements on the corrugated Cu_3N network reveal appearance of position dependent unoccupied electronic states in the energy range of 1.5-4.0 eV. LT-STS measurements were also performed for the atomic nanowires. The data show appearance of two electronic states at ~ 2 eV and ~ 4 eV. A trend of decreasing distance between the states has been observed with the increasing length of the nanowires. This observation will be discussed in view of the electronic structure of the Fe, Au, Cu/Cu_3N/Cu(110) system.

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29 SEPT. | 15:00 | Poster Session

Fermi surface and electronic structure of Sb(110)

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The electronic structure of systems characterized by strong spin orbit splitting is of fundamental interest in solid-state physics and relevant for applications in spintronics. In fact, in the last five years a new field has emerged from the understanding that the spin orbit interaction can lead to topological electronic phases in complex materials. Much of the fundamental physics of spin-split topological states had previously been discussed in connection with the simple surfaces of the semimetal Bi. The surfaces of Sb offer similar advantages as those of Bi, but with a much weaker spin-orbit interaction.

Here we report a combined theoretical and experimental investigation of the Sb(110) electronic structure. Measurements of the Sb(110) electronic structure were performed by combining scanning tunnelling microscopy and spectroscopy with angle-resolved photoemission. The results are compared to first principles calculations. We find several surface states close to the Fermi energy. The reduced strength of the spin-orbit splitting generally leads to a flatter dispersion of the bands compared to Bi(110).

Dynamic Correlations of the 3D and 2D Electron Liquid

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To date, understanding the dynamics of fermionic many-particle systems forms a major challenge for both experimentalists and theorists. For long wavelengths, Landau's concept of elementary excitations provides a powerful tool, leading to the well-known two types of modes: the collective ,,plasmon" mode, plus a continuum of incoherent particle-hole excitations. At higher wave vectors, the plasmon enters this band and is strongly damped. There seemed to be little room for further surprises in this field.

However, recent experiments [1] performed on a monolayer of liquid 3 He report the first observation of a roton-like minimum in a Fermi liquid. The collective mode reappears as a well defined excitation beyond the particlehole band. We explain this as a two-pair effect and predict a similar re- emergence for the plasmon. At the large wave vector (i.e. low energy) edge of the particle-hole band the collective modes regains substantial strength.

Our manifestly microscopic formalism is based on variationally optimizing time-dependent fluctuations of the wave funcion. We derive dynamic effective interactions and show how the form of the density-density response function must be changed from the RPA (random phase approximation) paradigm. We use state-of-the-art results for the static ground state structure as input and present results the for bulk as well as the two-dimensional electron liquid.

This work was supported by the FWF under project nr. P21264-N20.

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Growth of magnetic nanostructures on self-organized substrates

CAMINALE Michael[1], MORONI Riccardo[2], ANGHINOLFI Luca[1], BISIO Francesco[2], CANEPA Maurizio[1], MATTERA Lorenzo[1]

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INTRODUCTION

The sensitivity of localized surface plasmon resonances (LSPRs) to external stimuli has recently attracted a great deal of interest since it paves the way to the exploitation of plasmonic nanostructures for detection and to the possibility of tuning the optical functionality of plasmonic devices [1]. Having in mind this second objective, magnetic field has been recently proposed to modify the properties of surface plasmons and consequently to control the operation of plasmonic devices through the magneto-optical (MO) activity of the materials which form the device [2]. For this purpose the use of ferromagnetic metals, possessing large MO activity even though with plasmonic resonances usually broader and weaker then those observed in noble metals, can be envisaged. Alternatively, nanostructures made by combining noble metals and ferromagnetic materials can be used in order to take advantage of both the sharp LSPRs of the former and the large MO activity of the latter.

Here we investigate the possibility of using self-organized nanostructured templates for the preparation of nanostructured Fe film and array of Fe nanowires. In particular attention will be focused on the optical and magnetic properties of the samples.

MATERIALS and METHODS

We exploited self-organization processes occurring during the homoepitaxial growth on LiF(110) to obtain templates with periodic nanoscale ripple morphology [3]. We find that the wavelength of the ripple structure, consisting of coherently aligned {001} facets, can be controllably varied in the 15-60 nm range by varying the deposition condition during the homoepitaxial growth. The nanostructured LiF(110) templates thus obtained have been used as substrates for the growth of Fe nanostructured films and of arrays of Fe nanowires (Fig 1).

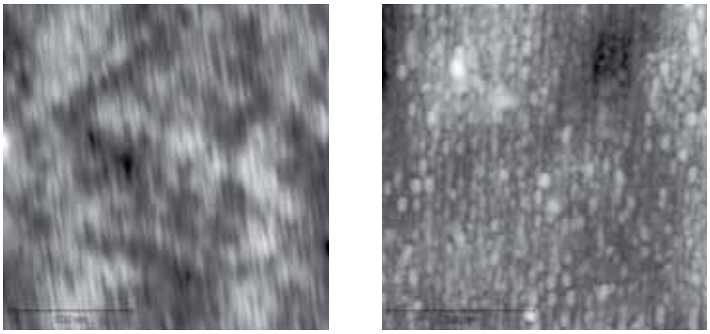

Figure 1: AFM views of the nanostructured LiF substrate (left panel) and of the Fe nanowires (right panel).

Nanostructured Fe films have been obtained by normal incidence deposition of Fe [4]. Fe nanowires have been obtained by exploiting shadowing effects occurring for grazing-incidence deposition on the nanostructured substrate [5,6] while control of nanowire size was achieved by varying the Fe coverage. In order to prevent oxidation, a 50 nm-thick LiF capping layer has been deposited on the samples, thus obtaining metallic nanostructures embedded in an homogeneous insulating host: an ideal system where to isolate the Fe contribution to the overall optical and magnetic properties. For this purpose, reflectance spectra have been measured with a variable angle spectro-ellipsometer (VASE) while magnetic hysteresis loops have been measured by magneto-optical Kerr effect (MOKE) measurements.

RESULTS and DISCUSSION

The reflectance spectra of the nanostructured film are slightly anisotropic (birefringent) due to the film anisotropic corrugation and essentially show a metallic behaviour. At variance, larger optical anisotropy and reflectance spectra typical of structures exhibiting LSPRs are observed for the nanowire sample. An attempt to model the dielectric function, and then the optical response of the nanowire systems, is achieved employing Effective Medium Approximation models, taking into account the finite size of the wires.

Hysteresis loops measured along and perpendicularly to the ripple direction point out a uniaxial magnetic anisotropy with easy axis parallel to the ripple direction for both the samples. Higher coercivity and higher anisotropy are observed for the nanowire samples. Moreover, for grazing incidence deposition, it was observed a strong dependence of the coercive field on the Fe coverage, with an abrupt increase in the initial deposition stages (1-3 nm) and the reaching of a saturation value (~1100 Oe) in the 4-6 nm Fe equivalent thickness range. This behaviour could be explained by the transition from isolated elongated Fe nanoparticles to continuous nanowires. Otherwise, for normal incidence deposition, the coercive field and the hysteresis loop shape, reaches a steady state (~300 Oe) soon after an Fe equivalent thickness of about 2 nm.

The larger coercive field of nanowires samples with respect to the one of the nanostructured Fe film is compatible with the establishment of different mechanisms of magnetization reversal (coherent rotation or curling in place of DW motion) while the increase in magnetic anisotropy shifting from the continuous nanostructured film to nanowires is qualitatively in agreement with the results of μ-mag simulations.

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29 SEPT. | 15:00 | Poster Session

Unoccupied quantum well states in ultrathin cobalt films studied by two-photon photoemission

CHIANG Cheng-Tien[1], WINKELMANN Aimo[1], HENK Juergen[1], YU Ping[1], KIRSCHNER Juergen[1]

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Unoccupied quantum well states in cobalt films on Cu(001) are investigated by spin and angle-resolved two-photon photoemission (2PPE) experiments.

In 2PPE experiments, the characteristic energy dispersion of quantum well states as a function of film thickness is observed [1]. This agrees nicely with previous result by inverse photoemission [2,3] and our first-principles calculations [4].

The 2PPE process via quantum well states shows strong variation upon sample magnetization reversal [1]. On the 7 monolayer cobalt film, this gives rise to a magnetic dichroism of 10% with linearly polarized light. The measured thickness dependence of magnetic linear dichroism allows us to connect the observed effect to the quantum well states.

In the spin-resolved 2PPE measurements, we observed a dominant majority spin polarization, extending from the initial states at 1.4 eV below the Fermi level up to the Fermi level. Moreover, we resolved an enhancement of spin-polarization by about 10% in 2PPE through the majority quantum well state in a 6 ML cobalt film. This is further confirmed by a cobalt thickness dependent measurement.

In combination with relativistic band structure and photoemission calculations [4], we demonstrate a systematic analysis of spin-orbit coupling in the unoccupied electronic structure of ferromagnetic cobalt films.

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Some quantum mechanical aspects of frictional force between parallel metallic slabs

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It is well known that the energy of a charged or neutral particle (e.g. electron or atom) at rest or slowly moving close to the dielectric surface, e.g. parallel to a metallic slab [1-3], is shifted downward, because of their interaction with the quantum mechanical charge density fluctuations in the system via nonretarded Coulomb interaction (at close distances), leading to dynamical image or van der Waals potentials, respectively. Parallel velocity leads to a typical "Doppler shifted" frequency in the resulting expressions.

For higher velocities real electronic transitions in the slab can occur and a moving particle starts losing kinetic energy. This dissipative phenomenon is well understood and described e.g. in terms of classical friction force, or complex potentials. In a way, it could be compared to the Brownian motion of the moving particle, which produces electric fields that are not translationally invariant, and the parallel momentum of scattered electrons in the metallic slab is not conserved. So the particle can transfer parallel momentum (and dissipate energy) to collisions with electrons in the metal.

In the last decade much attention has been paid to a similar phenomenon, namely frictional forces between two parallel dielectrics moving at parallel velocity, at zero temperature [4-8]. In this situation an obvious question can be posed: *Which mechanism is now responsible for friction, since translation symmetry is not broken (as was the case in the previous situation)?* This problem gave rise to a controversy, which is still alive [7,8]**,** in spite of much detailed work, e.g. by Persson et al., based on the original arguments in Ref. [4].

In this work we clarify some of these dilemmas, following Refs.[4-7], and extend the theory to include the effects of both collective and single particle excitations on the frictional force, using our earlier results for the van der Waals potential [9]**.** Theory is formulated for nonrelativistic relative velocities between slabs, but we shall demonstrate its extension to the retarded case when radiation losses can also occur, and to the finite temperatures, connecting it to our microscopic theory of Casimir forces [10]**.**

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29 SEPT. | 15:00 | Poster Session

Excited electronic states on surfaces: effect of NaCl atomic layers on metals

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The dynamics of excited electronic states at surfaces is greatly influenced by the presence of adsorbates. Indeed, insulating layers can separate efficiently electronic states localized on surfaces from those of the substrate resulting in a change of their lifetime with the layer thickness [1].

We present a theoretical study addressing how ultra-thin atomic layers deposited on metal surfaces influence the behavior of electronic excited states. We have studied systems with one to four atomic NaCl layers deposited on a Cu(111) surface. A wave packet propagation approach is employed for the description of the electron dynamics [2]. Model one-electron potentials were calculated taking into account polarization, Coulomb and short-range screening interactions, as well as mutual polarization. We have obtained the energy, lifetime and resonant wave functions of the electronic excited states in the system. Our results allow the interpretation of the oddities of experimental results in this system, measured using time-resolved two-photon photoemission [3], via the analysis of the link between the state lifetimes and their character (localization inside the layer or outside in vacuum).

We have also studied how the electronic excited states in the NaCl/Metal system are further perturbed by the presence of the applied electric field in a scanning tunneling microscopy (STM) experiment (NaCl/Ag(111) system) [4-6].

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Electronic structure of the layered material $NbSe_2$. Formation of charge density waves?

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During the last decade great effort has been dedicated to study a charge density wave (CDW) instability in transition metals dichalcogenides (TMD) [1-3], in particular in $NbSe_2$. This kind of material presents a layered structure (Fig. 1), which provides a good scenario to formation of CDW. Developments in theoretical and experimental areas attempt to elucidate which is the main driving force that produces the instability. Recent results based on angle-resolved photoemission spectroscopy (ARPES) combined with a simple theoretical model to describe the band structure propose that the Fermi surface nesting is the origin of the CDW in this compound. However, other authors reject this statement and take into account other possible mechanisms as responsible for these phenomena, such as van Hove singularities, electron-phonon coupling, and local field effects. Within a theoretical framework based on a time-dependent density functional theory our work is focused on the study of the energy loss function, where two approaches have been taken into account. The first one is the well-known random phase approximation (RPA) and the second one includes local field effects in the calculation of the loss function. These approaches are applied to study the wave vector dependence of the response function along two symmetry directions of the first Brillouin zone, where some evidence of instability was previously suggested. The inclusion of inter- and intra-band transitions and the influence of local field effects are analyzed.

References:

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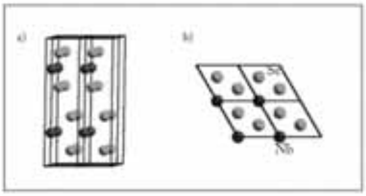

Figure 1 : Structure of $NbSe_2$ a) side and b) top view

29 SEPT. | 15:00 | Poster Session

Rabi oscillations in Time-dependent Density Functional Theory

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We have done a study of the Rabi oscillations in the semi-classical two-level approximation in the framework of Time-dependent Density Functional Theory.

The oscillations between the ground-state and the excited state can be observed in the time dependent dipole moment. By doing time dependent propagations on a one-dimensional system we were able to compare the behaviour of the exact solution with the results for different approximate functionals.

Molecular conductivity switching of two benzene rings under electric field.

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We study the electron transport and switching of S-C_6H_3F(CH3)-C_6H_3(CH3)F-S molecule sandwiched between two Au(111) electrodes using plane wave quantum transport calculation method described in [1-2]. A nonlocal pseudopotential method is used to describe the system, and scattering states are calculated. We found that under zero external electric field, the two rings have a perpendicular configuration, while under strong external electric field they change into a planar configuration. As a result, the quantum conductivity of the system will increase for more than ten times. We propose to use this as a molecular switch, serving the function of a transistor.

29 SEPT. | 15:00 | Poster Session

k-space based finite-size corrections for Quantum Monte Carlo calculations

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Computational methods for solids map the infinite system onto a finite system with periodic boundary conditions. Due to the long-range nature of the Coulomb interaction this leads to slowly decaying finite size errors. Mathematically one deals with a divergence at the Gamma point. The Quantum Monte Carlo (QMC) method is based on real space and several solutions exist: The real-space based Model Periodic Coulomb (MPC) interaction, a new k-space method introduced by Chiesa et al. (PRL 97, 076404, 2006) and our recent hybrid method that, using real space data, directly models the spherically averaged structure factor in k-space (PRB 75, 155105, 2007). We show that on integration our method exactly maps onto MPC and combines the best of both worlds. Furthermore, one can use known small |k| behaviour to improve convergence where MPC fails (e.g. slabs and surface like systems). The advantage of our method is that in contrast to k-space methods, one only deals with a simple single valued function that better lends itself to interpolation with exact small-|k| data as no directional information is needed. By virtue of integration the corrections can then be written as an addition to the MPC interaction.

Electron-phonon coupling in systems with strong spin-orbit interaction

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Surfaces and interfaces of materials with strong spin-orbit coupling have recently attracted considerable attention, not least because this interaction can lead to topological electronic phases in complex materials. In a simple two-dimensional Rashba system, the spin-orbit interaction (SOI) gives rise to a van Hove singularity in the density of states, in contrast to the constant density of states of a two-dimensional electron gas without SOI. It has been predicted that this singularity should have a noticeable effect on the electron-phonon coupling on the system [1].

We have tested these ideas by studying the temperature dependence of the electronic structure of a Bi/Ag(111) surface alloy, using angle-resolved photoemission spectroscopy. Bi, being a heavy metal, leads to pronounced spin-orbit coupling effects and these are even stronger in the surface alloy than for the clean Bi surfaces [2]. We analyze the self-energy for the entire surface state dispersion and find the expected increase as the temperature is raised. The electron-phonon coupling strength is, however, rather uniform over the tested energy range, suggesting that strong intra-band scattering to bulk states suppresses the expected enhancement of the electron-phonon coupling near the van Hove singularity.

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Dielectric response and optical properties of AlH_3 at high pressure

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Compressed hydrides have been the focus of many theoretical and experimental studies as candidates for high-temperature superconductors [1]. Indeed, these hydrides contain large fractions of H atoms and tend to be insulators at low pressure, while at high pressure they are expected to metallize. Since metallization of pure hydrogen has not been observed experimentally so far even at pressures as high as 340 GPa, these hydrogen-rich materials, which are expected to metallize at considerably lower pressure, are thought to be of relevance for studying phenomena related to metallic hydrogen. Metallization of the binary alloy aluminum hydride (AlH_3) was predicted at 73 GPa [2] and subsequently experimental evidence [3] of this phase was found.

In this work we report *ab initio* time-dependent density-functional theory calculations of the dielectric response and optical properties of the high pressure metallic phase of AlH_3 within the random-phase approximation. Low energy transitions between states near the Fermi level that appear in this metallized phase give rise to a low-energy electronic collective mode which is expected to induce an abrupt edge in the experimentally measured reflectivity just below 1 eV. An extension of our electronic structure study to a hypothetical system where only the H atoms are present and Al atoms have been replaced by a jellium background shows that AlH_3 is basically a hydrogen sublattice very weakly disturbed by Al atoms.

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Optical detection of plasmonic excitations in indium atomic wires: polarization dependence and annealing effect

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One-dimensional (1D) and quasi-1D electron systems has attracted much attention, because of their unique carrier transport as well as its collective charge-density excitation called 1D plasmon or Tomonaga plasmon. Such plasmon is expected when electrons in conduction bands are strongly confined in a narrow 1D object the width of which is similar to the scale of the Fermi-wavelength of the electrons. Among those quasi-1D electron systems, indium atom chains self-assembled on the Si (111) surface is one of the prototype systems for studying electronic and optical properties in atom-scale 1D objects. The In chain array forms 4x1 periodicity and can undergo phase transitions into a semiconducting phase with 8x2 periodicity at low temperature. This phase transition is induced by Peierls-type instability and has been studied by widely by many spectroscopic techniques. In this presentation, we usedour in situ infrared spectroscopy [1]to investigate the 1D metallic phase of this In chains, especially the nanostructure size dependence as well as polarization dependent optical properties by varying the annealing temperature. 1ML indium was evaporated onto Si (111) wafer with 1.8-degree miscut towards the [-1-12] direction. While heating up, RHEED patterns shows transformations from amorphous to small patches of multi-domain In 4x1 structure, and to single domain In 4x1 structure. The polarization-dependent spectra measured at room-temperature show a strong broad-band plasmonic absorption feature in the direction parallel to the wires, while in perpendicular direction the wires stay nearly transparent in the same spectral range.

In the parallel position, the infrared absorption peak shift from 2250 to 1200 cm-1 during annealing. It can be concluded that annealing can induce significant effect on the IR spectra. Corresponding high-resolution LEED spot profiles have also been taken to reveal the detailed domain size and structure evolution during annealing.

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29 SEPT. | 15:00 | Poster Session

An Iterative Method for Computing Molecular Absorption Spectra

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We present a fast parallel iterative method for computing molecular absorption spectra within TDDFT linear response and using the LCAO method. We use a local basis of ``dominant products´´ [1] to parametrize the space of orbital products that occur in the LCAO approach. In this basis, the dynamical polarizability is computed iteratively within an appropriate Krylov subspace. The iterative procedure uses a a matrix-free GMRES method to determine the (interacting) polarizability. The resulting code is about one order of magnitude faster than our previous full-matrix method [2]. This acceleration makes the speed of our TDDFT code comparable with codes based on Casida´s equation. The implementation of our method uses hybrid MPI and OpenMP parallelization in which load balancing and memory access are optimized. To validate our approach and to establish benchmarks, we compute spectra of large molecules on various types of parallel machines.

The methods developed here are fairly general and we believe they will find useful applications in molecular physics/chemistry, even for problems that are beyond TDDFT, such as organic semiconductors, particularly in photovoltaics.

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Photoemission from solids at low and high light intensities

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Theoretical approaches to angle-resolved photoemission from solids within and beyond the perturbation limit will be reviewed. The new generation of high intensity light sources has opened wide perspectives in solid state spectroscopy.Two main directions are being developed: multi-photon processes and attosecond time-resolved photoelectron spectroscopy.

A generalization of the one-step theory of photoemission to the second-order perturbation theory and its application to Si(001) will be presented. Multi-photon spectroscopy is demonstrated to be promising for studying momentum-resolved band-structure of unoccupied electronic states of bulk continuum.

Recently, first time-resolved measurements with subfemtosecond resolution have been performed for solids by laser-assisted photoemission, in which an ultra-short pulse of extreme ultraviolet radiation (XUV) creates a photoelectron wave packet with a temporal spread within a fraction of the oscillation period of the laser light. The energy shift of the photoelectron spectrum caused by the acceleration by the laser field as well as the distortion of the line shape provide information about the temporal structure of the excitation process. A phenomenological model will be presented based on a quasi-classical description of the interaction of the wave packet with the laser field. The model explains and quantitatively describes modulations of the width and center of gravity of the photoelectron spectra depending on the time delay of the laser pulse relative to the XUV pulse.

29 SEPT. | 15:00 | Poster Session

Electron transfer at ice/metal interfaces: Solvation dynamics at alkali-ion/water complexes

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Electron transfer across interfaces is of vital importance in various areas of physics, chemistry and biology. We have studied the dynamics of electron transfer and solvation processes in amorphous D_2O layers on metal surfaces using femtosecond time-resolved two-photon-photoemission (2PPE) spectroscopy. In these experiments, photoinjection of electrons from the metal into the adsorbate conduction band is followed by ultrafast localization and solvation of the excess electrons. The subsequent energetic stabilization of these solvated electrons (300 meV/ps) due to nuclear rearrangements of the polar molecular environment is accompanied by an increasing degree of localization. The population of solvated electrons decay non-exponentially with an initial decay time of 100 fs which slows down to several 100 fs with ongoing solvation.

Recently we have studied the influence of sodium and cesium ions bound near the ice –vacuum interface on the electron salvation dynamics. Adsorption of sub-monolayer coverages of sodium on top of multilayers of amorphous ice leads to the formation of Na^+ ions and to pronounced changes in the observed dynamics compared to pure amorphous ice. A new species of long-living electrons can be observed which exhibits much longer lifetimes of the order of 1 - 5 ps and faster energetic stabilization of 800 meV/ps compared to solvated electrons in pure D_2O ice. We attribute this species to a transient electron-sodium-ion-complex which is located at the ice/vacuum-interface. This interpretation is corroborated by coverage dependent measurements and by overlayer experiments.

Furthermore we have investigated the dynamics of the unoccupied alkali resonance of Na/Cu(111) and Cs/Cu(111). Coadsorbing small amounts of water enabled us to follow the energetic stabilization of the resonance upon the build-up of a solvation shell around the alkali atom containing up to 20 water molecules per atom. This stabilization is accompanied by an increase in the lifetime of the resonance.

Poster Session | 15:00 | 29 SEPT.

Dynamics of localized spin impurities in one-dimensional wires

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Recent experimental advances open up new possibilities for the research in spin dynamics with very high spacial and temporal resolution. The most representative examples include almost full control over individual spin-states in diamond [1] and manipulation of magnetic structures atom-by-atom using the scanning tunneling microscope, combined with the possibility of measuring spin-excitation spectra of individual atoms [2]. It has also been demonstrated that the magnetization dynamics can occur on a sub-picosecond time scale [3] giving access to ultra-fast phenomena involving spin.

Along with experimental advances there is an increasing need for theoretical understanding of the dynamics of the spin-degrees of freedom at atomic length and time scales, and fully atomistic time-dependent simulations are becoming a valuable tool for modeling spin dynamics at these limits.

In this work, we have applied a mixed quantum-classical Ehrenfest scheme for spin dynamics [4] to a model system consisting of two localized spins connected by a a finite mono-atomic chain. In our time-dependent simulations, an external spin-excitation is produced over one of the localized spins. It is then propagated by the itinerant spin-carriers along the chain, forming a complex pattern of spin-density evolution, and is detected in the dynamic response of the second spin. We have shown that by applying an electrostatic gate one can tune the effect of a spin-excitation in the chain coupling two localized spins and, therefore, induce different dynamic regimes in the system.

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29 SEPT. | 15:00 | Poster Session

Effects of asymmetric dipolar interactions between elliptical ferromagnetic nanomagnets in artificial spin-ice structures

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At the present time, arrays and networks of closely-spaced, dipole-coupled, single-domain nanomagnets are being intensively studied. The dipolar interactions between nanomagnets can be utilized to form a so-called 'artificial spin-ice' structure, which has been recently offered a novel approach to understanding and exploiting the properties of disordered systems. We demonstrate that dipolar interactions in such arrays can be exploited to induce and control magnetization states and reversal paths in nanomagnets that are completely different from those occurring in isolated nanomagnets.

We fabricated and studied arrays of elliptical ferromagnetic (material Py 25 nm thick) nanomagnets, and characterized them using our MOKE setup and Magnetic Force Microscopy (MFM).

The magnetic measurements show that the magnetization reversal process in the nanomagnets changes substantially by applying the external magnetic field parallel to (within ±0.2º) or at an angle from one of the sides of the squares forming the array. The simulations confirm this behavior: in this second case the formation and rotation of a so-called 'S' single domain state is observed in all the nanomagnets, whereas in the first case the formation of a so-called 'C' state, which evolves into a single vortex state, is observed in the two elliptical nanomagnets having their short axis parallel to the field.

We analyzed the role played by each of the nanomagnets in the magnetization reversal process, finding that the formation of the vortex state in the two nanomagnets with short axis parallel to the field is due to the asymmetry of the stray field generated by the other two nanomagnets in the spin-ice unit cell.

Confirmation of the existence of these intermediate metastable states was obtained using MFM after applying a suitable field sequence.

Our studies demonstrate that it is indeed possible to control the magnetization states in elliptical ferromagnetic nanoislands by placing localized magnetic field sources in their proximity, which can be easily facilitated within an appropriate array structure.

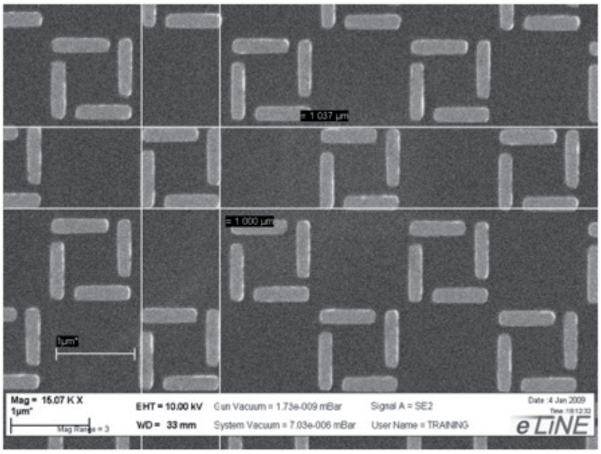

Fig.1: SEM image of the fabricated and analyzed sample.

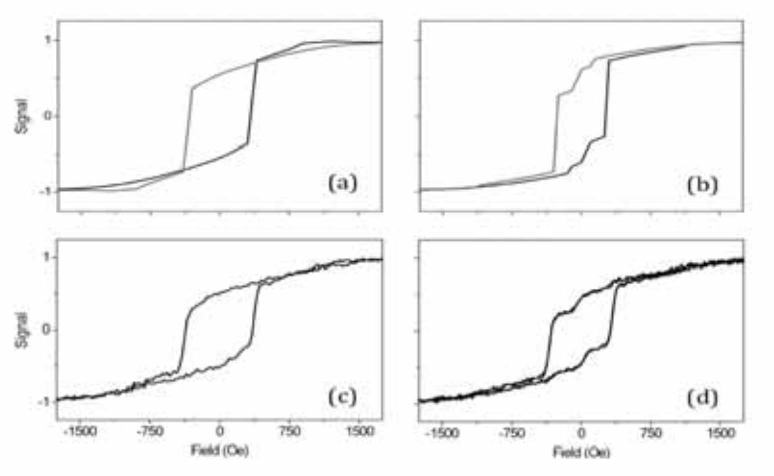

Fig.2: Calculated longitudinal-MOKE hysteresis loops for the off-axis (a) and on-axis (b) external applied magnetic field, and the corresponding measured hysteresis loops for the off-axis (c) and on-axis (d) cases.

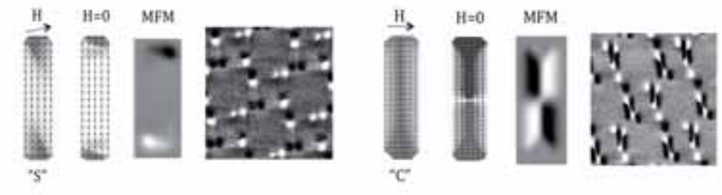

Fig.3: Calculations of the seed and remanent (H = 0) magnetization states in an interacting nanomagnet and the corresponding calculated and measured MFM images for the off-axis (left) and on-axis (right) directions of the applied magnetic field.

Computing the non-interacting electronic response function using Wannier interpolation

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Obtaining the non-interacting electronic response function of bulk systems or surfaces is a key step in describing their collective electronic excitations.

Computing this response function from ab initio can be an extremely demanding numerical task because the necessary sum over the first Brillouin zone must be performed on a dense mesh; this is especially true when studying low frequency features.

We propose a novel method for computing the response function which utilizes maximally localized Wannier functions [Phys. Rev. B 56, 12847 (1997), Phys. Rev. B 65 035109 (2001)]. While their construction requires the ab initio eigenvalues and wavefunctions on a relatively coarse reciprocal space "k" mesh, they can be used to interpolate the necessary input to the response calculation on a very dense "k" mesh. The numerical cost of this procedure is but a small fraction of the cost of performing a full non-self consistent ab initio calculation.

In essence, the Wannier procedure produces unitary "gauge" transformations over the band indices which, when applied to the coarse mesh wavefunctions, yield plane wave matrix elements which are maximally smooth. These matrix elements are then susceptible to standard interpolation schemes, which would otherwise have been ill-conditioned because of the arbitrary (and physically irrelevant) phase differences between different eigenstates. In turn, the band structure is obtained from Fourier interpolation.

In this talk we will also present results when the method is applied to various systems of interest where it becomes interestingly competitive.

Phonon-transport confinement effects in ridges investigated by electric means

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We have investigated experimentally the effect of lateral confinement of acoustic phonons in silicon ridges as a function of the temperature. In particular, the electrical 3ω method is used as a mean to generate phonons in 100nm large nanostructures and as a thermometer that allows tracking the heat flux generated. The determination of the mean free path of phonons as a function of the frequency remains a key point due to the consequences for heat transport and thermal management. Here we focus on the role of acoustic phonons in thermal conductivity, in the frequency range above 1THz. For a direct measurement of the averaged mean free path as a function of the temperature we have fabricated nanostructures consisting of silicon ridges on silicon substrates. The ridge top is a wire made either of metal or of doped silicon acting as a heater and as a thermometer in the same time. The lower part is an etched silicon substrate. This structure enables the generation phonons in the ridge and allows measurements of the heat flux flowing to the substrate.

In particular, an adaptation of the 3ω method is used to heat the wire. A model links the wire temperature to the heat flux transmitted to the substrate. In addition to the localized heat source effect, we investigated experimentally the consequences of the source not being a proper heat bath at equilibrium. We have successfully quantified the effect as a function of the two associated Knudsen numbers, namely the constriction Knudsen number describing the transmission of the phonons and the nanostructure Knudsen number characterizing the non-equilibrium of the source.

29 SEPT. | 15:00 | Poster Session

Double photoemission on superconductors

VOSS Stefan[1], WALLAUER Robert[1], JAHNKE Till[1], CZASCH Achim[1], HAVERMEIER Tilo[1], KREIDI Katharina[1], SCHMIDT-BOECKING Horst[1], SING Michael[2], CAMPUZANO J. C.[3], CLAESSEN Ralf[2], DOERNER Reinhard[1]

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We investigate the angular resolved single photoemission (ARPES) and double photoemission (DPE) from a Pb(111) crystal and Bi2212 in the normal and superconducting state (SC) using a coincidence detection method developed for gas phase experiments. It is a momentum resolved technique (often referred to as COLTRIMS) where charged particles are guided by homogeneous fields onto a position and time-of-flight sensitive detector consisting of micro channel plates and a delay line anode. While we find dispersion and the known band structure in the single photoemission spectra, correlated electron pairs do not show aomparable structure in momentum space. For photon energies above 25eV on Pb the DPE current is dominated by Auger-processes involving the 5d(5/2) and 5d(3/2) core levels emitting Auger-electrons of no specific angular dependence.

Wave intensity fluctuations in small disordered systems

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The statistical properties of wave transport through diffusive media have long been a topic of large interest and relevance to fields from astrophysics or “white paints” to electronic transport in mesoscopic media. Most of the work has been focused on the diffusive and localization regimes where the system size is much larger than the mean free path. The most useful theoretical approach that takes into account both multiple scattering effects as well as the system size is the (Dorokov-Mello-Pereyra-Kumar) DMPK equation. The statistical properties of a thin slab ("building block") of length dL has been recently derive [1] from a potential model and used to find the evolution with length of the expectation value of different physical quantities. It was found that the corresponding statistical properties of the full system depend only on the mean free paths and on no other property of the slice distribution. The universality that arises demonstrates the existence of a generalized central-limit theorem. However, these results were restricted to quasi-one-dimensional (Q1D) geometries.

Here we present a detailed analysis of the statistics of wave (light or electrons) intensity fluctuations and correlations in the limit when the system thickness is much smaller than the mean free path. The results of extensive numerical calculations are in good agreement with analytical results based on perturbative expansions. The extension of this perturbative approach to study wave transport through disordered thin films without the Q1D constrain will be discussed.

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Phys. Rev. E 7**5,** 031113 (2007).

P-029

Local investigation of fs-laser induced defects on Ag(100)

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It is well known that high power fs-laser create surface defects and even severe material restructuring in metal targets. This process has found its application in different laser processing techniques using laser fluences of 10^3 J/m to 10^7 J/m. We will discuss defects that originate manly from fs-laser induced hot electrons at laser fluences as low as 10 J/m. We use a low temperature scanning tunneling microscope to investigate this onset of laser defect creation on Ag(100). Our setup allows studying sample areas in the nanometer range directly before and after laser illumination and thus correlating the newly created defects to the local environment. In this contribution, results on defect type and density versus adsorbed laser fluence are presented.

Ab initio study on bulk Pb dielectric response and quasiparticle inelastic lifetime.

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Low-energy electronic excitations are known to play an important role on several properties of metallic systems, i.e., supeconductivity or optical constants. Here we present *ab initio* calculations results on the bulk Pb dielectric response (electronic collective excitations) and quasiparticle damping rates -or equivalently the inelastic lifetime- (single particle excitations) on the low-energy range. As lead is a heavy element, we study the spin-orbit coupling (SOC) effects on both the dielectric response and quasiparticle inelastic lifetimes.

First, a general analysis of the different features in the calculated energy-loss function will be given, showing their dispersion dependence on the momentum transfer direction and the role of local-field as well as SOC induced effects. The existence and nature of modes with characteristic sound-like dispersion is discussed, showing that even if Pb is a free-electron-like metal, a true acoustic plasmon should only exist for momentum transfers belonging to some reciprocal space directions.

Secondly, the quasiparticle damping rates results are reported. Screening as well as final states effects are analyzed in detail. A general quadratic dependence on the quasiparticle energy is found, thus showing a 3D Fermi liquid [1] behaviour. However, a more careful analysis shows the existence of bandstructure effects. Strong localization effects are also found. Last, an interesting link to quantum-well states (QWS) damping rates is shown, according to Refs.[2,3].

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29 SEPT. | 15:00 | Poster Session

Lifetime of quantum well states in Pb overlayers

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In supported metallic Pb thin films valence electrons behave as free-particles in the direction parallel to the surface, whereas confinement conditions (vacuum at one side and reflective barrier at the interface) in the perpendicular direction lead to the electron energy quantization.

These electronic states, known as quantum well states (QWSs), have been probed experimentally by scanning tunneling miscroscopy (STM) and photoemission (PES), demonstrating their characteristic properties [1]. Developments both in sample preparation and in experimental techniques, specially the time-resolved two-photon-photoemission, have lead to the accurate determination of the electronic structure and characterization of the electron (and hole) decay mechanisms of QWSs. Recent experimental studies [2-6] on extended Pb islands grown on different metallic and semiconductor substrates illustrate the current interest in this field.

In this work we extend a previous study [7] on lifetimes of QWSs of supported Pb films on Cu(111) by including the effect of the STM tip on the lifetime broadening. Our study combines both many-body techniques and wave packet propagation calculations, in the framework of one-dimensional pseudopotentials.

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Infra-red renormalization of the cross section and survival probability for scattering of image-potential band electrons from adsorbates

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Two-photon photoemission (2PPE) studies of electron dynamics in the quasitwo-dimensional image potential state (IS) bands on Cu(100) surface showed that the presence of small concentration of randomly distributed adsorbates may significantly affect the dynamics of quasiparticle propagation in surface bands[1]. In particular, simple theoretical analyses of the experimental data showed that the adsorbate coverage of the order of a percent gives rise to IS-electron scattering cross section in the range of few Å. Subsequent theoretical studies of the IS-electron scattering from adsorbates, and of the corresponding initial state survival probabilities, have revealed three distinct intervals of quasiparticle evolution and decays. These can be classified as[2]: (i) initial ballistic propagation regime and Zeno decay, (ii) consecutive period of Fermi-golden-rule (FGR) governed exponential decay, and (iii) crossover to a combined asymptotic power law and logarithmic decay. All three regimes are governed by the electron-adsorbate scattering cross-section and the ensuing properties of quasiparticle spectrum. The latter acquires logarithmic singularity at the IS-band bottom in all approximate calculations of quasiparticle self-energies in which, following the standard procedures[3], only the terms linear in the concentration c of the scattering centres are retained. This infra-red logarithmic singularity leads to a discrepancy between the measured and calculated cross-sections at low electron excitation energies. In the present work we remedy this deficiency by carrying out renormalization of the infra-red portion of the quasiparticle spectrum to all orders in c and thereby obtain better agreement of the calculated electron-adsorbate cross-sections with those observed in 2PPE experiments.

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29 SEPT. | 15:00 | Poster Session

PASSION FOR INTERFACES

ABSTRACTS

Organic and inorganic semiconductor interfaces across physics, chemistry and time

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Our understanding of the fundamental properties of solid surfaces and interfaces have seen a great development in the last 30 years due mainly to some experimental developments such as synchrotron radiation and the scanning tunneling microscope. Inorganic semiconductor interfaces will be quickly reviewed in this talk with special emphasis on their physical and chemical properties, such as electronegativity, charge neutrality level and metal/semiconductor barrier height. Organic interfaces will be discussed in more detail considering the metal/organic junctions formed between Au and C_{60}, TTF, TCNQ or PTCDA. The “organic energy gap problem” will be addressed, as well as the concept of the charging energy of the organic molecule: these quantities will be related to each other and to the metal/organic interface barrier height; examples for different organic/Au interfaces calculated using a first-principles DFT approach will be shown. The connection between the molecular (or the nanocontact) and the monolayer limits for these organic/metal interfaces will also be discussed. Finally, organic/organic interfaces will be reviewed using the concepts of the organic charge neutrality level and the interface screening.

30 SEPT. | 09:00 | Keynote Lecture

First-principles simulations of oxide hetero-structures: electrostatics, interface charges and vacancies

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The results of first-principles simulations will be presented for nano-scale structures of perovskite oxides. Results for nano-scale multilayer perovskite oxide heterostructures will be presented, mostly related to thin layers of lanthanum aluminate (LAO) on strontium titanate (STO). After the work of A. Ohtomo and H. Y. Hwang [Nature 427, 423 (2004)], electrostatic effects in such heterostructures have been shown to originate very interesting and potentially very useful effects. (001) interfaces of two different perovskite structures appear to give rise to intrinsic delta doping, which induces the formation of a two-dimensional electron gas when beyond a critical thickness of LAO. There is a need to push our understanding beyond the simple picture of electrons from the surface of LAO being transferred to the interface with STO, since, among other considerataions, (i) although a 2D electron gas is observed at the interface, no hole gas is seen at the surface; (ii) the number of carriers in the interfacial 2DEG is much less than expected; (iii) Core level spectroscopies indicate presence of electrons in the Ti 3d conduction bands at the interface beyond a critical thickness that is lower than the one for conduction; (iv) the expectation of a potential difference across the film that increases with film thickness is contradicted by experiments. Among the many papers steadily appearing on the subject, we will offer some insights gained from our simulations and simple models, on (i) the electrostatics of the problem, (ii) the net doping to be expected, and (iii) the effect of oxygen vacancies in the observed behaviours under increasing LAO thickness, addressing the open questions posed above.

*Work done in collaboration with N C Bristowe and P B Littlewood

Structure of self-assembled monolayers of alkylthiolates on Au(111) and Ag(111): a comparative study based on Density Functional and post Hartree-Fock calculations

BUSNENGO Heriberto Fabio[1], ABUFAGER P.N.[1], SOLANO CANCHAYA J.G.[1], WANG Y.[2], ALVAREZ SORIA L.[3], ALCAMÍ M.[2], MARTÍN F.[2], REUTER K. [4], MARTIARENA M.L.[3]

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We present a comparative study of the relative stability of various structures of high coverage (standing-up) self-assembled mono-layers (SAMs) [1] of alkylthiolates, $S(CH_2)_{n-1}CH_3=SC_n$, on Ag(111) and Au(111) based on: i) Density Functional Theory (DFT) calculations to evaluate the S-substrate interaction and ii) a chain-chain interaction potential, recently derived from second order Møller-Plesset (MP2) calculations for alkanethiols in gas phase [2]. For both substrates we consider the two possible surface coverages observed experimentally for Ag(111) and Au(111): i.e. $\Theta=3/7$ and $\Theta=1/3$ respectively.

For SC_1/Ag(111), we report a new possible structure for $\Theta=3/7$, involving top-most layer surface Ag atom vacancies (more stable than the most stable one found so far, corresponding to the unreconstructed surface) characterized by various structural parameters in excellent agreement with experiments [3]. Our calculations successfully account for the coverage observed for the shortest chain alkylthiolates as well as the experimental tilt angle of longer chain alkylthiolates on both substrates [1].

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Spin-spin and spin-orbital coupling effects at metallic interfaces

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The interaction of a magnetic adsorbate with a metallic interface usually brings about a reduction of the spin magnetic moment and a drastic change of its magnetic anisotropy. The reverse may be true for metal-organic complexes, where substrate-molecule charge transfer can give birth to a spin, couple it to another, and leave the magnetic anisotropy substantially unaffected. Using a combination of scanning tunnelling microscopy and x-ray magnetic circular dichroism, we study the spin and orbital moments as well as the easy magnetization direction of metal-organic complexes at surfaces, showing how much they are affected by hybridization with the substrate, ligand fields, many-body Kondo phenomena, and molecule-molecule interactions.

Atom-Specific Spectroscopy of Interfaces for Biosensors and Solar Cells

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The attachment of complex molecules to surfaces has evolved from a hap-hazard process to a sophisticated, multi-step process. This evolution has been particularly striking for biomolecules in biosensors. Antibodies need to be attached to a passivated surface in the optimum orientation to react with a protein or a virus. Single-stranded DNA needs to reach out from the surface to be accessible in DNA microarrays.

The multi-step biochemical reactions involved in the immobilization of proteins and DNA are now accessible to synchrotron-based soft X-ray spectroscopy. This interface-sensitive technique is able to detect specific bond orbitals at specific atoms. And the polarization dependence provides the orientation of the orbitals.

At a less sophisticated level, such methods are now put to good use in the design of molecule-based solar cells, an inexpensive alternative to semiconductor-based solar cells for large-scale photovoltaic arrays.

30 SEPT. | 11:40 | Invited Lectures / Oral Contributions

Single Molecule Spectroscopy: Electronic state, vibrational state and spin state

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Spectroscopy of single molecules at metal surfaces is nowadays available using scanning tunneling microscope (STM). Ultimate spatial resolution of STM even enables us to observe the inner electronic, vibrational [1-5] and spin [6] structures of a molecule adsorbed on solid surfaces. Vibrational spectrum of a single molecule provides useful information not only for the chemical identification of the molecule [1] but also for investigating how molecular vibrations can couple with the relevant dynamical processes [2, 3]. The response of vibrationally mediated molecular motion to applied bias voltage, namely an “action spectrum”, can reveal vibrational modes that excited through STM inelastic tunneling processes, because the molecular motion is induced only *via* the inelastic tunneling processes [4]. Thus, the action spectrum would be a candidate for detecting which vibrational mode is actually excited and associated with molecular motions. The mechanism to excite vibrational modes of molecules is revealed to be a resonant mechanism [5]. Life-time of the vibrational excited state was found to lengthen by inserting insulator thin film of MgO, decoupling the adsorbate and metal, enabled to split water molecule by exciting the OH stretching mode [7].
The ultimate spatial resolution in STS is utilized to characterize quantized state of carbon nano-tube at metal surface [8] and also the spatial distribution of defect state on TiO_2 [9].

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When energy is not a problem: interactions with fast and excited particles at surfaces.

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The fate of a chemical reaction is often determined by the availability of energy. Energy allows the reactants to overcome activation barriers and possible endoergicity of the reaction. The most probable path on the potential energy surface describing the reaction is also governed by availability of energy. In the case of excess energy, the potential energy surface can be explored much more efficiently. Regions of the surface above the ground state can be examined.

Control of reactant energy can be achieved by molecular beam techniques. Using these techniques we have recently studied the energy dependence of dissociation reactions at surfaces, such as H_2 dissociative chemisorption on (CO-)Ru(0001) and stepped Pt surfaces, the interaction of fast nitrogen radical atoms at metal surfaces, and Ar induced processes at CO-Ru(0001).

In the first example we could unravel the dissociation dynamics of hydrogen on basal planes of metals, on CO-covered Ru and on stepped Pt surfaces. A number of dynamic phenomena could be resolved thanks to the ability to vary the translational energy of hydrogen.

In the second example we make beams of the very reactive nitrogen atoms. We identified their adsorption and scattering from surfaces, and their interaction with pre-adsorbed nitrogen atoms. Strong non thermal and direct chemistry is observed. Also the first observations of the possible role of excited atoms has been made.

Fast Ar can energize a film of CO atoms and drive desorption and rearrangement of the film. Without sufficient energy the latter process is really problematic.

Achieving chemical accuracy for a prototype molecule-surface reaction

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Improving methods for computing the interaction of molecules with metal surfaces is critical to progress in modeling reactions on surfaces and heterogeneous catalysis. We introduce an implementation of the specific reaction parameter (SRP) approach to density functional theory (DFT) that allows the step forward from a semi-quantitative (conventional DFT) to a quantitative description of the molecule-surface interaction. Dynamics calculations on H_2 + Cu(111) using a SRP-DFT potential energy surface reproduce data on the reaction probability as a function of incidence energy and reactant state and on rotationally inelastic scattering with chemical accuracy [1]. However, the standard dynamical model used in these types of calculations (the Born-Oppenheimer static surface model) fails to accurately describe experiments on vibrational excitation of H_2, due to the neglect of the surface degrees of freedom. The SRP-functional derived for H_2 + Cu(111) also enables accurate dynamics results to be obtained for reactive scattering of H_2 from Cu(100).

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Mixed-valency signature in vibrational inelastic electron tunneling spectroscopy

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Density functional theory simulations of the vibrational inelastic electron tunneling spectroscopy (IETS) of O_2 on Ag(110) permits us [Alducin et al., Phys. Rev. Lett. 104, 136101 (2010)] to solve its unexplained IETS data [Hahn et al., Phys. Rev. Lett. 85, 1914 (2000)]. When semilocal density functional theory is corrected by including static intra-atomic correlations, the IETS simulations are in excellent agreement with the experiment. The unforeseen consequence of our calculations is that when adsorbed along the [001] direction, molecular O_2 on Ag(110) is a mixed-valent system.

Periodically Rippled Epitaxial Graphene: An Electronically and Structurally Nanostructured Material

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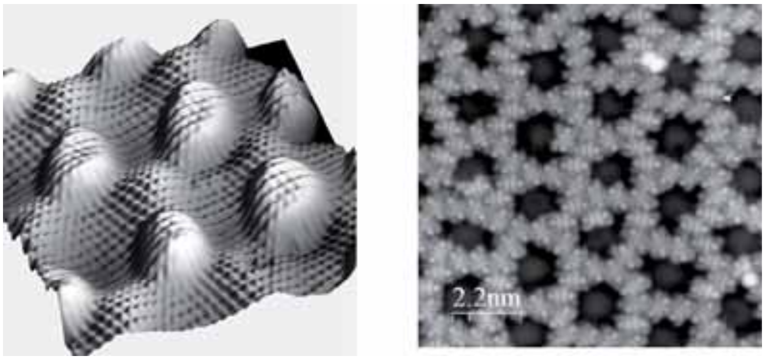
Graphene is an extraordinary material that allows a low energy manifestation of Quantum ElectroDynamics at surfaces. Its charge carriers behave as massless Dirac fermions with a group velocity ≈1/300 of the speed of light and display ballistic transport of charge and spin and a half-integer Quantum Hall Effect at 300 K.

Ultra perfect graphene monolayers, islands and ribbons can be epitaxially grown on many single crystal metal surfaces under Ultra High Vacuum conditions. These graphene layers are spontaneously nanostructured in a periodic array of ripples caused by the difference in lattice parameter between graphene and the different substrates. In-situ STM imaging of graphene monolayers grown on Ru(0001) or Ir (111) reveals that, in addition to the geometric corrugation, a much stronger electronic corrugation exists.

Local tunneling spectroscopy at 4 K shows that the rippled graphene layer consists in a periodic array of quantum dots containing electron and hole pockets. Electronic structure around the Fermi level, electron-phonon coupling, Image Potential States, Field Emission Resonances, doping and work function differences between “high” and “low” regions will be compared for epitaxial graphene on Ru(0001) and Ir(111). Examples will be shown of how these corrugated potential landscapes of epitaxial graphene provide with a periodic pattern that directs the self-assembly of different functional molecules on graphene. Implications of these findings towards a perfect atom mirror for a new Scanning Helium Atom Microscope and all-carbon electronic devices will be briefly discussed.



Atomically resolved STM image of ripples on epitaxial graphene grown on Ru(0001)(left) and TCNQ selectively adsorbed on it.

Single molecule manipulation by light and electrons

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The development of molecular switches on the single molecule level is a major challenge on the path towards incorporating molecules as building units into nanoelectronic circuits. Azobenzene derivatives are a prototype class of molecules that are well known to switch in the gas phase under illumination based on a cis-trans isomerization. With a scanning tunneling microscope (STM) it is also possible to induce this chemical reaction on an individual molecule by electrons tunneling inelastically from the STM tip into a molecule. We explored several azobenzene derivatives, p-hydroxy-azobenzene, amino-nitro-azobenzene, and anilino-nitro-azobenzene on a variety of surfaces, Cu(111), Ag(111), Au(111), and NaCl/Ag(111), in order to investigate the importance of the side groups and of the interaction strength with the surface. From these studies we deduce general rules for the feasibility of the use of azobenzene derivatives within nanoelectronic circuits.

Charging and electric field gating individual molecules at a hybrid metal-organic interface

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Electron transfer at organic-inorganic interfaces is conceptually difficult because the metal electrode is prone to interact chemically with the layer or act as a drain of charge. We will show that the localization of a single electron is, however, possible in molecular layers of the pure organic charge transfer complex tetrathiafulvalene (TTF) – tetracyanoquinodimethane (TCNQ) on a Au(111) surface. In these structures, the localisation of an unpaired electron in the LUMO of TCNQ leads to a free radical state, which can be demonstrated by the observation of the Kondo effect in low-temperature scanning tunnelling spectroscopy [1].

In the TTF-TCNQ system, the presence of a metal surface supports the charge equilibrium between donor and acceptor. This equilibrium, can however be manipulated by tuning the structure of the organic salt, as we found, for example, when we use tetramethyl-tetrathiafulvalene (TMTTF) as electron donor. TMTTF is electronically very similar to its parent TTF, but the four methyl groups slightly lift the electron donor backbone from the surface. The self-assembled monolayer with the acceptor TCNQ show essentially the same behaviour and most of the TCNQ molecules preserve their singly charged state as evidenced by a Kondo resonance. Interestingly, here it is possible to manipulate the charge state of the molecules using the tip of an STM. Tuning the magnitude of the local electric field we change the alignment of electronic levels, thus acting as a local gate that changes the charge state of an individual molecule.

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Adsorption of aromatic molecules: Tackling the van der Waals challenge with DFT-D?!

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The potential of a future molecular electronics has motivated many studies of functional organic molecules at metal surfaces. For first-principles theory it is particularly the possibly significant contribution of dispersive van der Waals (vdW) interactions in the molecule-substrate interaction that limits the common workhorse for large-scale calculations, density-functional theory (DFT) with semi-local exchange and correlation functionals. As higher-level theories including non-local vdW interactions by construction are presently barely tractable for corresponding system sizes, first insight could come from computationally inexpensive semi-empirical dispersion correction (DFT-D) schemes. There are relatively good reasons not to use present DFT-D formulations for adsorption at metal surfaces though. Using the adsorption of the molecular switch azobenzene at coinage metal surfaces as a case in point I will show that it sometimes doesn't hurt to proceed nevertheless.

Surface coordination chemistry: structure and reactivity of tetrapyrrole molecules

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The molecular functionalization of surfaces at the nanoscale is a key-point for designing novel devices as catalysts, sensors, solar cells, or molecular transistor, based on the interaction of an active surface with the surrounding molecular medium. In this context, metal complexes as porphyrins, phtalocyanines or corroles (tetrapyrrole molecules) are especially suitable because they combine the ability to form organized structures with an active site, usually a coordinated metal center. However, the high reactivity of some of these metal complexes enormously difficult its used and its functionality. An alternative route is to perform the coordination reactions directly on the surfaces which based on the importance of the surface-molecule interactions to form new complexes and how these interactions can promote the formation of ordered structures. One example is the metalation of the free metal molecules on surfaces by using vapour-deposited metal atoms. The routes reported in the literature for this surface mediated metalation in ultra high vacuum (UHV) conditions involve the evaporation of the metal atoms by vapor deposition in the proper stoichiometry (before or after the molecular deposition) and usually the annealing of the system formed by the substrate-molecule-metal atoms. The former procedure favors the metal atom diffusion and the subsequent coordination. Interestingly, in none of the reported cases, formation of complexes with the substrate metal atoms was detected. However, this possibility could simplify the surface synthesis of metalloporphyrins, since the step in which the metal atoms are added can be excluded. For example, protoporphyrin IX (H2PPIX) molecules adsorbed on cooper surfaces present the ability to form metallo-protoporphyrin IX (CuPPIX) even at room temperature (RT) in strongly bound self-assembled monolayers (SAMs).

From vacuum to atmosphere: microscopies and spectroscopies for molecular level studies of surfaces and interfaces

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The evolution of science is marked by the tools available to satisfy our curiosity. Telescopes allow us to see planets and stars. Optical microscopes to see cells. X-rays to determine the atomic structure of materials. When it comes to the “skin” of materials, the last few layers of atoms that constitute the surface, some of the most important tools are based on electron spectroscopies, scattering and diffraction. The key to surface sensitivity is the short mean free path of electrons and ions of moderate energy. With high vacuum technology these tools have made it possible to prepare clean and well defined surfaces, opening the way for studies of the atomic structure and dynamics. The past half century has witnessed enormous advances in the field through the systematic application of these techniques. However, these tools have reached an operational limit, because in many important applications the surfaces are exposed to gases near atmospheric pressure and liquids, which are opaque to electrons. Today we are crossing this pressure gap thanks to the development of a number of new techniques, including novel photon based techniques, and electron based techniques such as the Scanning Tunneling and Atomic Force Microscopes, and x-ray based photoelectron techniques. Through my career, curiosity has driven my research in many directions always related to surfaces: their atomic structure, how and where molecules adsorb, how they diffuse and react, what is the atomic level meaning of wetting and friction. I used any available tool to achieve my goals. When not available I developed them. I will illustrate with examples some of the topics that have excited my curiosity in recent years. These include molecular manipulation, diffusion and reactions, wetting at the nanoscale, friction and catalysis. For these endeavors the tools that I helped develop have been crucial.

Graphene interacting with transition metals: tuning the electronic and magnetic properties of graphene

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I will first present some recent results for the electronic structure of rippled graphene on Ru(0001). Using a combination of scanning tunnelling spectroscopy and ab initio density functional calculations we have explored the spatial variation of the unoccupied electronic states of graphene epitaxially grown on Ru(0001) [1]. Several unexpected features are observed: (i) the first graphene image state is split in energy, unlike all other image states; (ii) the split state does not follow the local work function modulation; (iii) and a new interfacial state at +3 eV appears on the lower areas of the rippled graphene layer. Our first-principles calculations explain these observations. On the one hand, the unexpected splitting of the first resonance is due to the confinement of the electronic states induced by the metallic substrate with a pronounced projected band gap around G in the relevant energy range. The upwards energy shift is larger for those areas of graphene closer to the surface and can overcome the opposite variation of the work function. Thus, the rippled graphene layer behaves as a self-organized periodic array of quantum dots. On the other hand, the new interfacial state corresponds to a surface resonance that, for the clean Ru surface, appears slightly below the edge of the Ru(0001) projected band gap. When the distance between the graphene layer and the Ru(0001) surface is smaller than 3.0 Å, this Ru resonance is promoted to a surface state and starts to hybridize with the first image state of graphene. The position of this interfacial state strongly depends on the graphene-metal distance and, therefore, can be eventually used to characterize this distance with high accuracy.

Next, I will present some surprises recently found for transition metals as substitutional impurities in graphene [2]. For example, from the traditional ferromagnets Ni, Co and Fe, only Co retains a spin moment of ~1μB as an isolated substitutional impurity in graphene (Co_{sub}) [2]. However, when the Co substitution takes place in more than one site, the total magnetic moment of the system exhibits a strong dependency on the relative position of the Co_{sub} impurities that closely resembles what is expected for simple vacancies in a π-tight-biding model of graphene according to Lieb's theorem for a half-filled bipartite lattice [3]. In particular, the total spin moment behaves as $|Co_{A-}Co_{B}|$, where Co_A and Co_B are, respectively, the number Co substitutions in the A and B graphene sublattices [4]. Ni_{sub} impurities, although non-magnetic for flat graphene, develop a non-zero magnetic moment in metallic carbon nanotubes [5]. This behavior stems from the peculiar curvature dependence of the electronic structure of Ni_{sub}. A similar magnetic/non-magnetic transition of Ni_{sub} can be expected by applying other kinds of anisotropic strain to a flat graphene layer.

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Graphene-covered iron layers on Ni(111): structural and electronic properties

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Recently, Dekdov et al. [Appl. Phys. Lett. 93, 022509 (2008)] reported the intercalation of atomic Fe layers between graphene and a Ni surface. In the present work, we report new experimental and theoretical results on this novel nanostructure. Fe intercalation was produced by repeatedly evaporating monolayers of Fe57 on previously prepared graphene/Ni(111), and post-annealing at 320 C. In situ Mössbauer spectra are consistent with a single hyperfine magnetic field for the one-Fe-monolayer system, while the two-monolayer system presented two field values. By using low energy electron diffraction (LEED) the strucuture of both graphene/Ni(111) and graphene/Fe/Ni(111) was investigated. The model that best fits the experimental LEED curves corresponds to one C atom on top of Ni or Fe and the other C atom on a *fcc* hollow-site, consistent with the most stable systems in the first-principles calculations. Regarding the calculated electronic structure of the studied systems, the graphene/Ni structure presents a bandgap of 0.06 eV for the minority-spin electronic states near the original graphene Fermi point. The inclusion of Fe layers modify the magnitude, and even the existence, of such bandgap. For instance, in the case of the one-Fe-monolayer system, the bandgap increases to 0.63 eV.

Ultra-high dense array of magnetic quantum dots on a $GdAu_2$ template

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The growth of magnetic nanoparticles on surfaces by auto-organization processes represents a flexible and powerful alternative to obtain high-density, patterned magnetic storage media. Here, we report on the growth of a dense array of magnetic quantum dots on a $GdAu_2$ surface alloy. We show that this $GdAu_2$ surface alloy behaves as an excellent template to achieve dot arrays with very high areal densities up to 54 Teradots/inch^2. The structural properties of the template and the tunability of the quantum dot array have been thoroughly explored by Scanning Tunneling Microscopy and X-ray Photoelectron Spectroscopy. The magnetic response of the magnetic quantum dots has been investigated showing room temperature remanent magnetization.

Electronic structure relations of oxide metal interfaces at the atomic level

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Planar oxide based model systems may be probed with surface science techniques leading to catalytically relevant knowledge of practical use. The oxide metal interface is of particular interest in catalysis. In this paper we highlight the influence of the thickness of oxide films, which are grown on metal single crystals, onto the properties of metal atoms and clusters located on the oxide film surface. It is shown that the thickness controls the charge state of the deposited metal. The main factors are the support metal-oxide interfacial ionization potential and the electron affinity of the deposited metal on top of the oxide film, together with its lattice response. We show also that such thin oxide films, which are models for the “strong metal support interaction” (SMSI) state of dispersed metal catalysts, may enhance reactivity, and may have potential to design new catalysts and understand existing ones. Also, model systems for so-called “monolayer oxide catalysts” are briefly mentioned.

28 SEPT. | 11:05 | Invited Lectures / Oral Contributions

Dynamic and static processes in interface interaction

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The interaction between adsorbates and substrate determines not only the surface structure but also the dynamical character of adsorbate motion and is key to understanding processes such as self-assembly. Observing the dynamics on length scales of a single unit-cell and on time scales that allow the intra-cell and inter-cell motion to be resolved is, however, a major challenge. We have recently demonstrated that surface systems can be explored in unprecedented detail using an adaptation of the spin-echo method applied to molecular beams of helium [1].

The results reveal energy landscapes that vary from the high corrugation, which is a characteristic of localized bonds in atomic species [2], to the flat, but surprisingly high friction, landscape observed with C_6H_6 on a graphitic substrate [3], illustrated in figure 1. The results suggest a direct connection between the lateral extent of an adsorbate and the dissipative character in the motion. The behaviour we observe shows the importance of metastable adsorption sites and provides new insights into the origin of inter-adsorbate forces. Finally, we have recently been able to obtain a direct, and quantitative, measure of the quantum contribution to the motion in the case of light adsorbates such as hydrogen and deuterium. The observations reveal that these light adsorbates experience an unusually strong frictional coupling, which cannot be explained by a simple phononic model of dissipation.

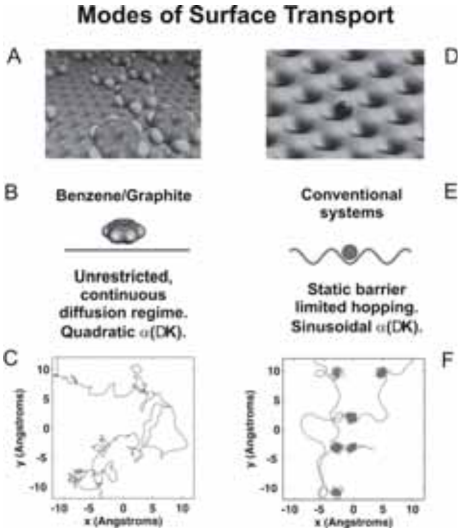

Figure 1. Surface transport in a high-friction viscous regime (a-c) and typical hopping motion (d-f).

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Theoretical investigation of the Eley–Rideal recombination of nitrogen on Tungsten(100)

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Among the different processes taking place at the gas-surface interface, molecular recombination play a decisive role. The theoretical description of such mechanisms is thus a fundamental goal in surface chemistry and physics.

Using the Classical Trajectory method, the dynamics of molecular recombination of nitrogen (N_2) from a Tungsten (W/100) surface is investigated, focusing on the Eley - Rideal (ER) mechanism. The study relies on a recently developed potential energy surface based on an extended version of the periodic London-Eyring-Polanyi-Sato (LEPS) function. The influence of surface temperature on the reacton dynamics is accounted for via the Generalized Langevin Oscillator (GLO) model.

Time-resolved investigation of laser-induced diffusion by optical second-harmonic microscopy

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A non-linear dependence on laser fluence is characteristic of many femtosecond laser-induced surface processes. It results in a strong variation of the rate across the laser beam profile, which requires either a profile-corrected analysis or a spatially selected detection.

Here, we report an experimental technique for spatially resolved optical second-harmonic generation (SHG), i.e. SHG-microscopy, to detect laser-induced adsorbate diffusion or desorption and their dependence on laser fluence. We illustrate its operation on the basis of a time-domain study of laser-induced diffusion of oxygen on a vicinal Pt(111) surface at low substrate temperature. In our SHG-microscopy experiment, the femtosecond laser pulses induce not only the diffusion process from the O-saturated steps onto the terraces via excitation of hot electrons but also generate second-harmonic light which is detected spatially resolved via an intensified CCD camera. Using the sensitivity of SHG on step coverage [1] and analyzing the signal change across the laser beam profile via SHG-microscopy, the strong fluence dependence of the diffusion process could be investigated.

The strong non-linear fluence dependence made it further possible to apply two-pulse correlation techniques to study the dynamics of the energy transfer between laser-excited substrate electrons to the adsorbate degrees of freedom. We observe an increase of the width of the two-pulse correlation from 0.8 ps to 1.7 ps when the laser fluence increases from 1.6 mJ/cm^2 to 3.7 mJ/cm^2. The results are discussed on the basis of an empirical friction model [2].

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'QM/Me' - a novel embedding approach for adsorbate dynamics on metal surfaces

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The dissociative adsorption of oxygen molecules on metal surfaces is a commonly known, highly exothermic reaction and in its slow or fast form of great importance for corrosion or oxidation catalysis, respectively.
However, knowledge about atomistic details of the heat dissipation, a central conceptual concern, is very limited at best. Even on the level of Born-Oppenheimer potential energy surfaces, accurate dynamical ab-initio descriptions of such reactions are quite challenging from a computational point of view: Modeling the excitations of substrate phonons within periodic boundary conditions requires huge super-cells, whereas traditional 'QM/MM' embedding schemes demand unfeasibly large metal clusters.

In the novel 'QM/Me' approach presented here, the adsorbate-substrate interaction is obtained from periodic first-principles calculations in convenient super-cells. This is combined with a 'bath-like' substrate based on classical potentials, which are parametrized to seamlessly fit the first-principles data. To illustrate our approach, we use the dissociative adsorption of oxygen and molecules on Pd(100) using density-functional theory and a modified embedded atom potential for the quantum and classical region, respectively. We observe dissipation of a dominant fraction of the released chemisorption energy into the bulk already on a picosecond time scale, analyze phonon excitations and discuss consequences for the adsorbate dynamics. With the so obtained accurate reference data, a critical assessment of 'heat sinks' from the literature, e.g. thermostats and the surface oscillator model, will be presented.

Electronic damping of vibrations: the case of NO on Au(111)

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When dealing with molecule-surface scattering, energy relaxation and line braodening are known to play an important role. For instance, it has been observed that a vibrationally excited NO molecule loses a significant amount of vibrational energy at the vicinity of a Au (111) surface[1]. This has been interpreted as a sign for the breakdown of the Born-Oppenheimer approximation due to vibration-electron coupling. We present the periodic density functional calculations that allowed us to obtain the ground state potential energy surface along the desorption and NO-vibration coordinates. Additionally, two different methods to calculate vibrational damping rates including the anharmonicities [2,3] are compared. They serve as an input for a time-dependent calculation including dissipation.

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Exotic Kondo effect in metalorganic complexes controlled by ion-substrate interaction

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The realization of bottom-up molecular spintronic devices requires precise control of the magnetic properties of single molecules at the interface with a metallic substrate [1,2]. Molecules belonging to the metal-phthalocyanine (MPc) family represent an ideal model system for this purpose, since their planar macrocyclic structure can basically accommodate all transition metal ions, allowing us to disentangle the effects of metal-substrate and ligand-substrate interactions.

Here we present a comparative scanning tunneling spectroscopy study of four different types of MPc complexes (M = Fe, Co, Ni, Cu) adsorbed on the Ag(100) surface. We study the magnetic properties of these molecules via the Kondo interaction with the substrate. In all previous studies of the Kondo effect in MPc and similar metalorganic complexes, the Kondo resonance arose from the interaction between the ion and the substrate, the ligand playing the role of controlling the coupling strength. In stark contrast, in our study we observe a Kondo resonance arising from the interaction of a ligand spin with conduction electrons. The interaction is controlled by the symmetry of the active d-states of the central ion. This anomalous behaviour, with inverted ion and ligand role, underlines the importance of considering the ligand as a direct participant of the magnetic characteristics of hybrid metal-organic structures.

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Interactions between H_2O and pre-adsorbed O or D on stepped platinum surfaces

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Platinum electrodes are often used in fuel cells, where water is the most commonly used solvent. Most studies modeling the Pt/H_2O interface use the low index Pt(111) surface as a model. Real catalytic surfaces, however, have a more complex geometry, containing low coordination or defect sites in addition to (111) terraces.

Two species that are often present along with H_2O in fuel cells are oxygen and hydrogen. Under UHV-conditions ("ultra high vacuum") on Pt(111) the co-adsorption of O or H binds water stronger to the surface. On O-covered surfaces this is due to OH-formation [1], whereas on H-covered surfaces this is arguably due to hydronium formation [2].

To unravel the influence of defects in the surface chemistry of Pt electrodes, we study co-adsorption of $H_2{}^{16}O$ with pre-adsorbed ^{18}O or D on a series of stepped Pt surfaces in UHV. We use temperature programmed desorption (TPD) in combination with isotope exchange. We show for the first time that the tendency for O_{ad} to be hydrogenated to OH by H_2O depends crucially on whether it is bound to a (110) or (100) step site or to a (111) terrace site. Our results suggest that oxygen adatoms are an alternative intermediate for step-mediated electrochemical oxidation reactions. For hydrogen co-adsorption, water is less strongly bound than to the bare surface, in contrast to what is observed on Pt(111). Surprisingly, we find that the step geometry determines whether the surface is hydrophilic or hydrophobic.

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Potential barrier mapping at metal-organic nanocontacts

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Electron transport through metal-molecule contacts greatly affects the operation and performance of electronic devices based on organic semiconductors and is at the heart of molecular electronics exploiting single molecule junctions. Much of our understanding of the charge injection and extraction processes in these systems relays on our knowledge of the potential barrier at the contact. Despite significant experimental and theoretical advances in our understanding of electron transport in molecular junctions, a clear rationale of the contact barrier at the single molecule level is missing. Here we exploit scanning tunneling microscopy to probe directly the nanocontact between a single molecule and a metal electrode. Contrary to the common assumption of a uniform barrier, we show here that this varies on the sub-molecular scale. Our experiments reveal that the local modulation, can amount to more than 1 eV across the 4-[trans-2-(pyrid-4-yl-vinyl)] benzoic acid molecule on the copper surface. This spatial dependence reflects the interaction between specific molecular groups and the metal and allows clearly visualizing the processes leading to the formation of a built-in interface potential. Furthermore, this barrier can be opportunely be manipulated by the formation of specific metal-organic nano-contact.

Barrier Formation and Charging Energy for Metal/Organic Interfaces. From the Monolayer to the Single Molecule Limit: C_{60}/Au(111) and C_6H_6/Au(111)

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New electronic devices, like OLEDs, based on organic materials have already appeared in the market. The performance of these devices depends critically on the energy barriers created between different organic and metal layers. These are determined by the relative position of the molecular levels across the metal/organic (M/O) or the organic/organic (O/O) interfaces[1,2].

Molecular level alignment at M/O junctions has been extensively studied[1,2]. The Schottky-Mott rule, based on the vacuum level alignment, has been disproved by the substantial interface dipole exhibited by many M/O junctions. In order to explain the alignment several models have been proposed. Of particular interest is the Induced Density of Interface States (IDIS) model[1], that is based on the tendency of the Charge Neutrality Level (CNL) of the organic material to align with the metal Fermi level due to the charge transfer between the two materials.

In this work we combine a DFT calculation of the structural and electronic properties of M/O interfaces with an analysis of the interface barrier formation based on the IDIS model[1]. It is well-known that in these systems it is necessary to go beyond standard DFT to properly describe the HOMO-LUMO gap and thus obtain a correct description of the electronic structure of the interface. Our analysis allows us to determine the charging energy (U^{eff}) of the molecule at the interface, correct the DFT transport energy gap and obtain a realistic metal/organic barrier height[3]. This method has been applied to the C_{60}/Au(111) and benzene/Au(111) interfaces for various coverages, from the monolayer to the single molecule limit. Realistic benzene-gold distances have been calculated including the Van der Waals interaction[4] in the DFT calculations of the interface.

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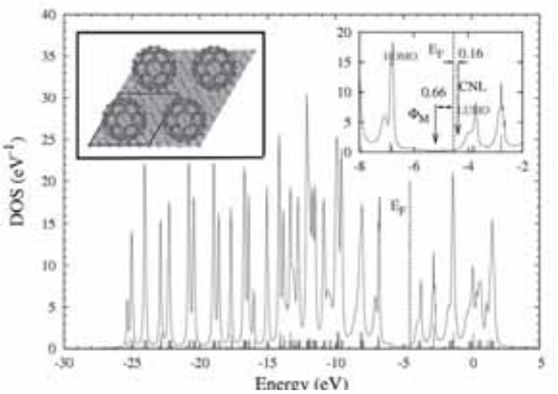

Figure 1: DOS proyected on the C_{60} orbitals for the C_{60}/Au(111) $2\sqrt{3}x2\sqrt{3}$ R30º monolayer shown in left inset. Right inset: Enlarged image for the area around the Fermi Level, showing HOMO, LUMO and CNL of the molecule, workfunction (Phi_M) of non-interacting gold surface and Fermi Level (EF) of the system. Note that E_F-Phi_M is the IDIS potential V^{IDIS}. The molecular levels for the C_{60} neglecting interaction with surface are shown as red vertical lines.

Fermi Gap Engineering by Au doping of the Ag/Cu(111) Dislocation Network

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Self-assembled metallic superlattices have attracted much attention in the context of nanoscale fabrication, due to their suitability for nanostructured templates with 1-10 nm periodicities. Ag/Cu(111) represents one of the most simple and promising metallic superlattices. The fact that this system features a surface state with a gap at the Fermi energy[1] makes it a suitable candidate for surface state nanoelectronics materials[2]. In this context, we present an Angle Resolved Photoemission Spectroscopy study of Au-doped 1ML and 2ML Ag/Cu(111) systems. The -point Fermi gap of 1ML Ag/Cu(111) system has been found to move smoothly below the Fermi level as a function of Au doping. The 2ML Ag/Cu (111) system does not reveal a gap below the Fermi level, but such gap arises with Au doping. Such control over the Fermi gap in 1ML and 2ML Ag/Cu(111) might open a new way for further application in the very same analogue to the graphene-based technology.

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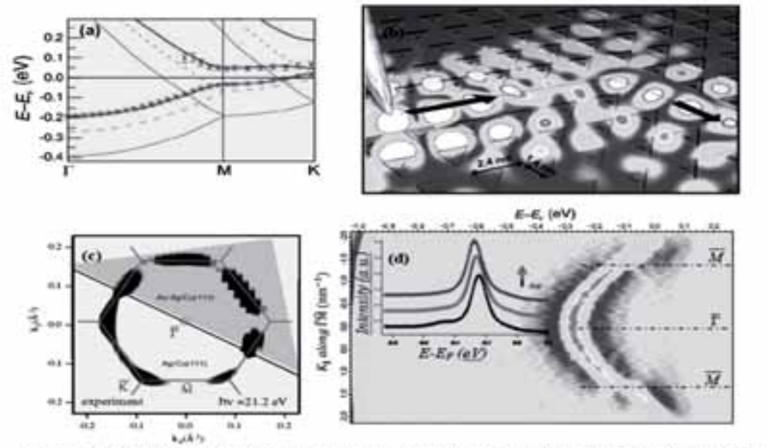

Figure: (a) Surface bands for Cu(111) (blue), a simple model band structure calculation of the 1ML Ag without triangular dislocations (dotted), with triangles (red), and experimetal photoemission data (symbols) for the triangular network [1]. **(b)** Principle of waveguiding and bending of electronic surface states (EESs)[2]. **(c)** Fermi surface of 1ML Ag/Cu(111) and Au doped Ag/Cu(111). **(d)** Surface state of 1ML Ag/Cu(111) doped with certain amount of Au and the corresponding energy distribution curves as a function of Au doping.

Nanofluidics and Tobacco Mosaic Virus?

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While microfluidic devices enjoy widespread popularity, the properties of fluids and flow processes at the nanoscale, especially for fluid confinement below 30 nm, are largely unknown. The main experimental hurdle is the design of channels that are chemically and structurally well defined down to (nearly) atomic dimensions. Taking advantages of the self-assembling properties of the Tobacco mosaic virus (TMV) particles, we build tube-shaped nanoobjects with a 4 nm internal channel and immobilize them on patterned solid surfaces using micro- and nanofabrication techniques. Finally dynamic fluidic experiment can be conducted exploiting the ability of an environmental scanning electron microscope (ESEM) to condense and evaporate liquids in-situ.

Vibrational dynamics of hydrogen on germanium surfaces probed by sum frequency generation spectroscopy

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Vibrational lifetimes of adsorbates are of crucial importance for many surface chemical processes [1]. The relaxation dynamics of local vibrational modes of adsorbates provides insights into energy decay processes to other vibrational modes and the substrate phonon bath. Here we present studies on the relaxation dynamics of the H-Ge stretching mode on Germanium surfaces by sum frequency generation (SFG) spectroscopy. Germanium can be seen as an interesting alternative to proof some concepts developed earlier when interpreting similar data for Si-H [2,3]. Our results are discussed with respect to possible relaxation schemes [4,5].

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29 SEPT. | 15:00 | Poster Session

Field Emission Resonances on periodically rippled graphene

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Moiré patterns are generated by the superposition of two periodic structures with a lattice mismatch. They have been observed by means of Scanning Tunneling Microscopy (STM) on different systems and their interpretation, in some cases, is not straightforward. The influence, at the atomic scale, of these patterns in the local density of states of the overlayer is not clear.

The growth of graphene on metallic substrates allow us not only control the periodicity of the moiré pattern but also tailor the interaction strength between the carbon atoms and the metallic substrates. This modulation in the interaction gives rise to regions with larger (H-areas) and shorter (L-areas) height of the graphene layer over the Ru(0001) surface. Field Emission Resonances (FERs), which are detected by STM when applying voltages larger than the work function, can be used to explore with nanometer resolution, the inhomogeneities in the local surface potential landscape. Operating the STM in constant current mode implies a constant electric field between tip and sample and the expected energy position for the FERs gives information about the surface potential.

The dZ/dV curves measured on gr/Ru(0001) present three unexpected features: (i) the first graphene image state is localized on the H-areas, while it is more extended on the L-areas, (ii) it does not shift in energy following the 0.25 eV increase of local work function from L- to H-areas, and (iii) a new interfacial state at +3 eV appears in the L-areas. To further investigate and understand the origin of these features we performed first principle calculations based on density functional theory. Our calculations explain the experimental data as consequence of the splitting and spatial localization of quasi-two dimensional bands due to the modulation of the strength of the interaction between the graphene layer and the metal surface.

The effect of surface motion on H_2 dissociation on Cu(111)

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The correct prediction of elementary processes occurring when H_2 scatters from a metal surface is one of the main challenges in the field of heterogeneous catalysis. The reactive scattering of H_2 on Cu(111) has often been used as prototype system. This is because of two reasons: quantum dynamics calculations using a model that includes all degrees of freedom of the hydrogen molecule are feasible and are expected to give a reliable description of many experiments, and a great number of experimental results is available. Recent six dimensional quantum dynamical calculations reproduced reaction probabilities measured in molecular beam experiments, initial-state resolved dissociation probabilities, and data on rotationally inelastic scattering with chemical accuracy [1]. However still some refinements of the model are needed to get a proper description of vibrationally inelastic scattering of H_2, and of the rotational quadrupole alignment parameter of reacting D_2. To this purpose, we plan to include the surface motion in the description of the system, both in the Potential Energy Surface (PES) and in the dynamics. As a first step, we systematically investigated how the motion of the surface atoms affects some features of the PES, such as the dissociation barrier height and the geometry corresponding to some representative reaction pathways and the anisotropy of the potential with respect to the angular coordinates of H_2. This analysis allowed us to choose the single surface degree of freedom that is likely to be most relevant for H_2. dissociation. We extended the PES developed by Díaz and co-workers [1] to include this surface motion, and we will study the dynamical effect of this surface motion by means of 7D quantum dynamics.

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29 SEPT. | 15:00 | Poster Session

Interfacial contributions stabilizing polymer solutions

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It is well known that at the optimal conformation condition polymers in solution present a free energy minimum very weak due to the balance between opposite driving forces: the enthalpic contribution, due to the unit local interaction, and the entropic one, governing the extent of its states in the phase space. The water wetting the biopolymers build up an interfacial region surrounding each polymer nanoparticle (NP) that match the external solvent phase and the NP core region. The NP finite size makes this interfacial contribution very relevant to the equilibrium free energy of each solute in solution. In this work we presents a systematic study on poly-oxyethylen-glycol polymers (PEO) undergoing different constraints: i) free PEO polymers in solution at different molecular weight, ii) PEO polymers constituting the hydrophilic termination of C12Ej surfactant at a given length of the hydrophobic termination (11 CH_2 groups and one CH_3; C_{12}), but varying the the hydrophilic chain length from 5 to 8 E units ($E=CH_2-CH_2-O$), iii) PEO polymers bounded on gold NP. Our results combine analysis of mass density measurements, compressibility, molecular dynamic simulations, small angle neutron scattering, neutron spin echo. Under all the constraints the main properties of each unit (volume, bound conformations) remain the same, and the helix conformation is preserved. Analyzing the micellar core volume we observed that besides the Laplace extra pressure due to the finite size, there is a contribution proportional to the percentage of hydrophobic interface directly exposed to water.

Modelling Polar Complex Oxide Heterostructures

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Complex oxide heterostructures not only offer the potential for exciting new physics but also the opportunity to replace conventional semiconductor devices due to reduced (nanoscale) feature sizes and added functionality. We present a theoretical study, using first principles calculations and phenomenological modelling, of two prototypical polar complex oxide systems:

a) $LaAlO_3/SrTiO_3$

The two-dimensional electron gas (2DEG) discovered at the insulator-insulator LAO/STO interface has since been found to be switchable and exhibit an insulating to metal transition (IMT) with film thickness. We address the origin of the 2DEG and its properties.

b) $(La,Sr)MnO_3/BaTiO_3$

The room temperature half-metallicity of LSMO makes it an attractive option for spintronics. The discovery of nm thick ferroelectric BTO films on an LSMO substrate introduces the possibility for multiferroicity. We attempt to address the origin of the stability of ferroelectric BTO films and its influence on the interface magnetism of LSMO.

Water Adsorption on Clean and Oxygen Decorated Ru Surfaces

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Water growth on metal surfaces has been a topic of debate during many years. Nowadays, it is still unclear what are the growth mechanisms and the structures for water layers on many substrates. An important ingredient to understand the self-organization of water in metallic surfaces is the competition between inter-molecular and metal-substrate interactions. This competition determines whether the molecules (i) cluster in a 3D-phase, (ii) wet the surface following a well-ordered 2D-adlayer or even, in a more complicated scenario, (iii) a significant fraction of water molecules in the layer should undergo partial dissociation (thus, decomposing into H and OH).[1-3]

Both, the inter-molecular and metal-substrate interactions, are strongly influenced by the substrate itself and by co-adsorbing other adsorbates.[4] In this work we have explored the importance of the cooperative effects in the adsorption of water on clean and oxygen decorated Ru(0001) surfaces using Density Functional Theory (DFT). For low oxygen coverage (up to 0.25 ML), we observed a significant reinforcement of the intermolecular hydrogen-bond (H-bond) for small water clusters. This H-bond is accompanied by the red-shift of the O-H stretching mode of the donor molecule. This enhancement of the H-bond can be attributed to the polarization of the donor molecule when bonded to the Ru atoms in the substrate.[5]We also consider the impact of the H-bond strengthening in the barriers for partial dissociation of water.

At higher oxygen coverage, consistent with the O(2x1)/Ru(0001) surface, we present a combined low temperature scanning tunneling microscopy (STM) and DFT study of the adsorption of water on the Ru(0001) surface pre-covered with 0.5 ML oxygen. The adsorption of water causes a shift of half of the chemisorbed oxygen atoms from hcp sites to fcc sites, creating a (2x2) honeycomb structure. Our calculations show that the energy cost of reconstructing the oxygen overlayer is more than compensated by the adsorption of water on the newly created unbounded Ru atoms. The STM images reveal a (4x2) water super structure, which is due to the existence of two relative orientations of the water molecules. Heating to 185 K results in the complete desorption of the water layer. Interestingly, the oxygen honeycomb structure induced by the adsorption of water remains metastable after water desorption and does not revert to the stable linear 2x1 structure until after temperatures close to 300K.[6]

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Organic Donor-Acceptor Assemblies on Au(111) Surface

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Organic electronics has become an enormously promising field of technology due to the prospect of size reduction offered by molecular-level control of the relevant material properties. However, many challenges have still to be overcome before this technology becomes mature and commercially competitive, requiring first a thorough understanding of the basic science involved in the operation of organic electronic devices and the physics of organic semiconductors. Of particular interest and relevance for the performance of organic electronics, we find the various interfaces present in the devices, where such crucial processes as e.g. charge injection take place.

Within this frame, we focus here on intermolecular and molecule–substrate interactions in model donor–acceptor assemblies at metal-organic interfaces, namely, fluorinated copper-phthalocyanines (F_{16}CuPC) and pentacene (PEN) assemblies on the Au(111) surface. In order to explore such interactions, a variety of techniques has been used, such as scanning tunneling microscopy (STM), x-ray standing waves (XSW), near edge x-ray absorption fine structure (NEXAFS) and x-ray photoemission spectroscopy (XPS).

By these techniques, we obtain a full picture of the crystallographic and electronic structure of PEN and F_{16}CuPC monolayers as well as of their binary mixture on the Au(111) surface. From the STM crystallographic analysis, we observe a long-range ordered crystalline structure for the binary mixture which can be traced back to the greatly enhanced intermolecular interaction via hydrogen bonds. Interestingly, the new supramolecular structure involves changes in the electronic structure of the molecular components. In particular, as observed by XPS, the changes affect the F_{16}CuPc, while no effect has been observed on the PEN. This difference can be regarded as an indication of the different interactions between the acceptor (F_{16}CuPC) and the donor (PEN) with the Au(111) substrate in the mixed state.

29 SEPT. | 15:00 | Poster Session

Tilt-angle dependent conductance of thiol- and amino-terminated SAMs over Au(111)

FOTI Giuseppe[1], FREDERIKSEN Thomas[1], SANCHEZ-PORTAL Daniel[1, 2], ARNAU Andrés[1, 2, 3]

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We investigate the conduction through different SAMs between gold electrodes using the *ab-initio* DFT code TranSIESTA based on the Non-equilibrium Green´s function formalism (NEGF). The transport properties of the molecular junction are studied as a function of tilt angle, anchoring groups and length of the molecules.

We observe a tilt-dependent "molecular gate effect" which is responsible for a relatively large change of the conductance. Moreover, as we increase the tilt angle, due to the presence of intermolecular pathways between neighbouring molecules, longer chains show higher conductance enhancements. We confirmed these results for thiol- and amino-terminated chains. As a notable difference, we expected a much stronger renormalization of the energy levels in the case of NH_2 as terminal group, respect to sulfur, related to a much higher (and opposite in sign) charge transfer mechanism between molecule and gold surface. We have performed calculations in order to confirm this expectation.

The PDOS over different atoms of the scattering region allows us to estimate the contribution of each kind of atom to the final transmission coefficient of the junction as a function of energy and tilt angle.

Using a toy model of the SAM under study (including anchoring groups and adatoms) in the tight-binding approximation, we get an insight into the physics behind the origin of the peak in the transmission coefficient of alkanedithiols with the tilting of the molecule.

Theory of SP-STM applied to local spins

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We provide a theory for scanning tunneling microscopy and spectroscopy using a spin-polarized tip. It it shown that the tunneling conductance can be partitioned into three separate contributions, a background conductance which is independent of the local spin, a dynamical conductance which is proportional to the local spin moment, and a conductance which is proportional to the noise spectrum of the local spin interactions. The presented theory is applicable to setups with magnetic tip and substrate in non-collinear arrangement, as well as for non-magnetic situations. The partitioning of the tunneling current suggests a possibility to extract the total spin moment of the local spin from the dynamical conductance. The dynamical conductance suggests a possibility to generate very high frequency spin-dependent ac currents and/or voltages. We also propose a measurement of the dynamical conductance that can be used to determine the character of the effective exchange interaction between individual spins in clusters. The third contribution to the tunneling current is associated with the spin-spin correlations induced by the exchange interaction between the local spin moment and the tunneling electrons. We demonstrate how this term can be used in the analysis of spin excitations recorded in conductance measurements. Finally, we propose to use spin-polarized scanning tunneling microscopy for detailed studies of the spin excitation spectrum.

29 SEPT. | 15:00 | Poster Session

Transport properties of fullerene nanocontacts

FREDERIKSEN Thomas[1], SCHULL Guillaume[2], BERNDT Richard[3], BRANDBYGE Mads[4], SANCHEZ-PORTAL Daniel[1, 5], ARNAU Andrés[1, 5, 6]

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Controlling the transport of charge through molecular structures is essential for future electronic devices based on organic materials. In recent years techniques to study single-molecule junctions have rapidly advanced, leading to new insight into the conduction mechanisms. Important challenges today include a determination of how atomic-scale variations in the molecule-metal interfaces influence the junction conductance and a characterization of the charge transport from one single molecule to another one.

In this talk I describe our combined experimental and theoretical efforts to understand these aspects for transport through C60 molecules studied with a scanning tunneling microscope. With the ability to prepare C60-functionalized STM tips [1] we first characterize transport through a single C60 molecule by bringing the tip into contact with Cu atomic clusters of different sizes assembled on a Cu(111) surface. We find that for clusters consisting of only a few atoms the conductance depends critically on the cluster size. However, for larger clusters the conductance stabilizes to a value effectively limited by the nature of the molecule and its interaction with the metal [2]. Secondly, we also use the C60-tips to make contact to another C60 molecule adsorbed on the Cu(111) surface. In this way we study intermolecular charge transport in a C60-C60 bridge geometry. We find that the bridge conductance is not sensitive to the metal-molecule interface but rather limited by the interface between the two molecules.

First-principles transport simulations reproduce the experimental data, allow a detailed characterization of the junction geometries, and identify the essential roles of the molecule-metal and intermolecular link in the conduction process. The theoretical analysis thereby provides insight into the limiting factors for transport in C60 junctions.

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Catalycity from first principles: atomic and molecular oxygen processes over ZrB_2 (0001) surface

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Ceramic materials are frequently used in spacecrafts (e.g., Space Shuttle) thermal protection systems (TPS) mainly due to a high temperature resistance, a low weight, among other technical important properties. The study of the atomic and molecular oxygen heterogeneous processes involved over these materials is important to design appropriate TPSs [1]. The mechanisms and the reaction rates of these air-surface processes in such hypersonic flows are not well known even at room temperature and it is very important due to their high influence on the TPS degradation and on the total heat transfer to the vehicle. This heat release depends on γi and βi (i = OO, NN, NO,...) coefficients, the atomic recombination coefficient and the chemical energy accommodation, respectively. The aim of this work is the calculation of these coefficients using first principles and kinetic models.

With this purpose, we have studied the interaction of atomic and molecular oxygen over the ZrB_2 (0001) surface [2], for both boron and zirconium termination, by means of Density Functional Theory calculations to understand much better the behavior of ZrB_2-based materials in the presence of pure oxygen and air hypersonic flows. Stationary points (e.g. adsorption minima) and energy barriers for the main elementary heterogeneous processes are obtained. Thermal rate constants for atomic adsorption, Eley-Rideal and Langmuir-Hinshelwood reactions and molecular (dissociative and non-dissociative) adsorption have been obtained by means of Transition State Theory in the 100 K - 1500 K temperature range. All the rate constants obtained have been included in a typical kinetic model [3] with the aim of obtaining the variation of surface coverage for all the species involved with time, taking into account about ten elementary processes. Calculated γi (T,P) coefficients for different total and partial pressures will be presented and discussed at the meeting.

ACKNOWLEDGEMENTS
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29 SEPT. | 15:00 | Poster Session

Molecular Vibrations during the Formation of Metal-Molecule Nanocontacts

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In recent years, charge transport through metal-molecule systems has become a major subject of study within the field of nanoscale science. A main result of these studies is that the structural and electronic properties of the molecule can be significantly altered by the atomistic arrangement at the junction and the coupling between the molecule and the metallic electrodes. In particular, the effect of the metal-molecule coupling is stronger as junctions are tuned from tunneling to contact regime.

The strength of the metal-molecule coupling and its variation during the contact formation, can be characterized through the spectroscopic signal of the molecular vibrations as measured by inelastic tunneling spectroscopy (IETS). This can be recorded as a function of the tip-molecule distance allowing understanding to which extent the contact formation influences the molecular properties.

In this work, we combine IETS measurements with first-principles calculations to achieve a precise characterization of the metal-molecule interaction during contact formation. We use the IETS signal of a single CO molecule adsorbed on a Cu(111) metal surface. Both the measured data and the calculations show characteristic shifts of the vibration modes [1]. In particular, we observe a continuous but nonlinear blue shift of the frustrated rotation mode in tunneling with decreasing distance followed by an abrupt softening upon contact formation. This indicates that the presence of the metal-electrode sensibly alters the structural and conductive properties of the junction even without the formation of a strong chemical bond.

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Room Temperature Spin Transport through C_{60} molecules

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Organic semiconductors (OS) have extremely low spin-orbit interaction, so that the main spin scattering mechanism is thought to be the hyperfine coupling with protons [1,2]. Consequently, the electron spin diffusion length is expected to be very long, making OS ideal materials for spintronics. Recently, several experiments have been performed studying the spin injection and transport in organic semiconductors, focusing only on a relatively limited number of molecules [3].

Here, spin transport studies through C_{60} layers are presented. C_{60} is commonly used in organic transistors and in organic photovoltaics devices, while no spin transport experiments have been carried out with it so far. Nevertheless, it is an ideal molecule to study magnetotransport properties: it does not contain hydrogen atoms, thus minimizing the hyperfine coupling with protons. Hybrid $Co/Al_2O_3/C_{60}/Py$ vertical spin valves were produced, with the C_{60} layer thickness ranging between 3 nm and 30 nm, and an Al_2O_3 layer of around 2 nm between the bottom Co electrode and the C_{60} layer to improve the effective spin polarization at the interface [4].

AFM and X-ray reflectivity measurements show that C_{60} grows smoothly on the Al_2O_3 layer, with roughness below 2 molecular layers. The spin valve resistance-area product is constant for all the junctions grown in the same conditions, and increases exponentially with the C_{60} thickness. Magnetoresistance has been reproducibly measured at room temperature (see fig. 1), suggesting a room temperature spin relaxation length longer than 20 nm. We will compare these results with some of our recent studies in lateral spin valves with C_{60} channels.

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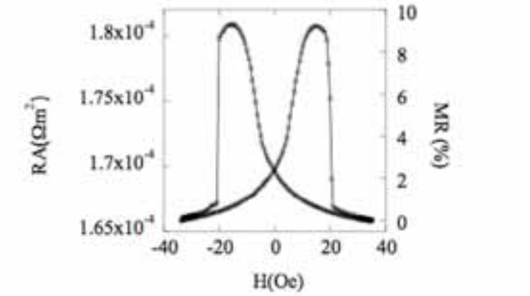

Fig. 1. Room Temperature magnetoresistance in a $Co/Al_2O_3/C_{60}$(5nm)/Py spin valve.

Adsorption dynamics of N_2 molecules on Fe(110) and on W/Fe(110) surfaces

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A comparative study of the adsorption dynamics of nitrogen molecules on Fe(110) surfaces and on monolayers of W on Fe(110) is done. On experiments [1] it has been shown that Fe(110) is a quite unreactive surface; however, this reactivity is substantially increased when a monolayer of W is put on Fe. Such a monolayer grows pseudomorphically. As the lattice constant of W is 9.4% larger than that of Fe, the Fe/W(110) surface is more open than that of Fe(110).

As a first step, the ab-initio Potential Energy Surface (PES) in six dimensions of both systems is calculated using DFT and interpolated using the Corrugation Reducing Procedure[2]. Later, classical dynamic calculations for different energies and incidence angles are made, and the probability of the molecules to dissociate, molecularly adsorb or reflect is consequently analysed. As a final step, non adiabatic effects as the electron-hole pair excitations within the local density approximation are studied [3].

According to the obtained results, a comparison of the reactivity of these two surfaces is made, concluding whether such a difference is due to structural or chemical effects.

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Self-Assembly of Donor-Acceptor Networks

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Synthesis of nanostructured donor-acceptor molecular mixtures is of great interest for the development of organic optoelectronic devices such as solar cells. Understanding the interactions that determine the crystalline structure of these molecular layers and interfaces is of great importance considering its intimate relation with the electronic properties and, as a consequence, with their functionality in devices.

Copper-phthalocyanine (CuPc, donor) and perfluorinated Pentacene (PFP, acceptor) are two semiconducting molecules well known for their successful integration into electronic nanodevices. In our study, these two molecules are deposited on metallic substrates separately as well as together, and the crystalline structure of the self-assembled molecular layers is studied by STM. Two different substrates of similar symmetry but different lattice spacing and reactivity have been used: Ag(111) and Cu(111).

In contrast to the relatively weak intermolecular interactions expected in single-component layers (dominated by van der Waals forces and steric effects), the formation and optimization of C-H···F-C hydrogen bonds in the binary layers is considered responsible for the growth of highly ordered donor-acceptor nanostructures. We observe virtually the same arrangement on both substrates, indicating that the substrate does not play a critical role and that it is mainly the intermolecular interactions that determine the molecular arrangement. However, the role of the substrate as a template cannot be wholly disregarded, since the observation of discrete rotational domains evidences in all cases epitaxial relations with the overlayer.

In addition to the crystalline information obtained by STM, a combination of synchrotron based high-resolution XPS and NEXAFS measurements provides valuable information on the effect of the distinct intermolecular interactions associated to each supramolecular environment (binary vs. single component layers) on their electronic properties.

29 SEPT. | 15:00 | Poster Session

Structure and electronic properties of TCNQ-F4 deposited on clean Au(111)

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Organic molecules with strong electron-accepting character such as tetracyanoquinodimethane (TCNQ) and its derivatives have been extensively studied in the last few years due to their unique properties when they are combined with other materials. For example, in combination with electron-donating organic species they form organic charge-transfer complexes that exhibit interesting optical properties for Organic Light Emission Diodes (OLEDs), photovoltaic response for solar devices, etc. In order to develop these devices the complexes must be combined with metallic surfaces, and thus their performance depends critically on the electronic and structural properties of the organic/metal (OM) interface.

In this work we study the adsorption of fluorinated TCNQ (TCNQ-F4) on the Au(111) substrate. Experimentally it has been observed that TCNQ-F4 molecules deposited on clean Au(111) readily self-assemble into large domains, where two features can be distinguished with a 1:1 ratio: spheres and ellipsoidal features. High resolution STM images allow proposing a model for the adsorption geometry, with ellipses interpreted as TCNQ-F4 molecules and spheres associated to Au adatoms released from the surface. DFT based theoretical calculations permit us to confirm this model by comparing experimental STM images with theoretical STM simulations, as shown in Figure1.

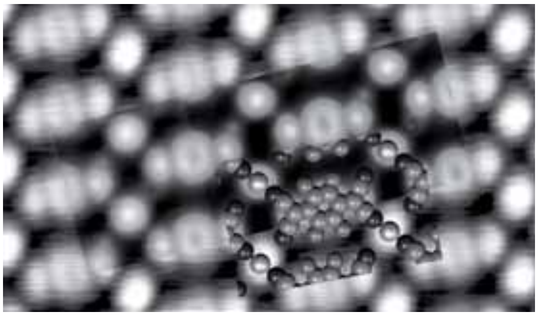

Figure 1: Composition of experimental STM image, theoretical simulation and structural model of the adsorption geometry of TCNQ-F4 on Au(111) including Au adatoms.

In addition to the structural model, STS spectra also show very interesting electronic features that clearly differ from the spectra taken on the centre of the molecules and the metal adatoms. Using different theoretical tools, like PDOS on molecular orbitals, induced densities, etc. we investigate the origin of these spectral features and unravel whether they are originated from a mixing of metal and molecular states, that is, whether they correspond to hybrid bands formed at the OM interface.

Spin-Orbit Coupling in Tl/Si(1,1,1) surface

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Since the rather unexpected discovery of spin-splitting of the Shockley type surface states this phenomenon has attracted considerable interest due to its relevance in the emergent field of spintronics. During the last decade, a great effort has been concentrated in order to produce and understand device functions based on the electron spin, where surface and interface studies play an outstanding role. We present an analysis of the effect of the spin-orbit coupling on the electronic surface states in the Tl/Si (1,1,1) surface, as a model system to understand the spin structure and spin-orbit coupling phenomena in surfaces and interfaces. Our calculations show the existence of two spin-split surface states crossing the Fermi level. These states form an effective two dimensional spin polarized electron gas due to the semiconductor nature of the Si substrate, the Fermi surface being completely defined by them. Among other quantities, we report the detailed electron/spin structure of surface electrons, providing the momentum dependent magnetization and energies of the relevant surface states.

29 SEPT. | 15:00 | Poster Session

Probing the scattering of N_2 from W(110) surface with different exchange-correlation functionals

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The rotational inelastic scattering of N_2 from W(110) is studied using classical molecular dynamics (MD). In a previous study of the dissociative adsorption of N_2 on the W(110) surface based on potential energy surfaces (PES) calculated with two different exchange-correlation (XC) functionals (PW91 and RPBE), it was shown that neither functional is able to get overall agreement with experiments [1]. Hence, this study stimulates our interest to make a comparative classical MD study based on the six dimensional-ab initio PES obtained with the above-mentioned XC functionals in order to investigate their results for the scattering of N_2 from W(110). For low incident energy of Ei=0.1eV and at normal incident angle, our results show that the PW91-PES is a good choice to determine the rotational distribution of the scattered molecules. On the other hand, for higher incident energies, Ei=0.5 to 1.0eV, at the same incident angle, the rotational distributions of the scattered molecules calculated from the RPBE- PES agree well with the experimental ones. Thus, our findings provide further evidence that the choice of the exchange correlation functional plays a key role for the accurate predictions of the dynamics of molecule/surface interactions.

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Dissociative adsorption dynamics of H_2 on a precovered Pd(100) surface

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We employ classical molecular dynamics calculations based on Density Functional Theory molecule-surface interaction potentials to study H-coverage effects on H_2 dissociative adsorption on Pd(100). We have found that at large coverages, H_2 molecules can still dissociate spontaneously even on a single isolated empty adsorption site, in contrast with one of the basic assumptions of the widely used Langmuir model.

We have also found that not only the global coverage is relevant, but for a given initial coverage, the particular arrangement of the ad-atoms on the surface plays a very important role in particular at very low energies. This shows that surface coverage alone does not provide enough information to predict and/or understand surface reactivities.

29 SEPT. | 15:00 | Poster Session

Theoretical study of non-reactive scattering of N atoms off Ag(111) surfaces

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During the last years, experimental progress has improved our understanding of gas-surface interactions. In spite of this progress, it is still difficult to extract a full description of the dynamical processes from experimental results. On the other hand, the theoretical studies make it possible to analyze the dynamics of a wide range of processes, helping to the understanding of experimental data.

In this work, we investigate the non-reactive scattering of N atoms off Ag(111) surfaces. Our calculations rely on an accurate potential energy surface based on density functional theory (DFT) calculations. Interpolation of the DFT data is performed using the corrugation reducing procedure [1]. Dynamics is studied using a Monte Carlo sampling and classical trajectories. In particular, this study focuses on the angular and energy distributions of the scattered hyperthermal N atoms. Energy dissipation to the metallic surface through phonons is taken into account with the Generalized Langevin Oscillator model. Electron-hole pairs excitations are also included using a local friction coefficient [2]. Our theoretical results are in reasonable agreement with recent experimental data [3]. A detailed analysis of the dynamics is showed and the role of both energy dissipation channels is also pointed out.

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First-principles Adsorption Characterization of TTF, TCNQ and TTF-TCNQ on Au(111): Structural and Electronic Properties, Charging Energy and Theoretical STM

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The adsorption of a molecular electron donor/acceptor on Au(111) is characterized by the spontaneous formation of a superlattice of monomers spaced a distance ranging between several nanometers apart or that to form closepack monolayered structures [1]. Particularly, tetrathiofulvalene (TTF) and tetracyanoquinodimethane (TCNQ) are prototypical electron donor and acceptor, respectively, and are in potentials of molecular electronics. Accordingly, in their complex TTF-TCNQ a partial electronic charge will be transferred from the HOMO of TTF to the LUMO of the TCNQ. Therefore, TTF-TCNQ states as a promising candidate of organic conductor [2]. The adsorption of single TTF and TCNQ molecules, and their adlayered structures, on Au(111) has been systematically investigated. In our theoretical approach we first calculate the geometric configuration of the metal/organic interface as a function of the molecule-substrate distance and the molecule adsorption site by using a DFTLDA technique. The electronic structure and metal/organic barrier height formation for the single molecules, as well as for the adlayered structures, are analyzed by using the Induced Density of Interface States (IDIS) model [3] for metalorganic interfaces. Whitin this framework we calculate the charging energy Ueff of all the isolated and adlayered systems at the nanocontact, and determine selfconsistently the transport energy gap and the organic molecule density of states. The Ueff obtained from the analysis can be used to correct the Kohn-Sham energy gap as Et(gap)=EKS(gap)+Ueff(gap) by using a scissor operator, also employed to circumvent the poor description of the Au workfunction given by standard DFT via the correct levels alignment. Additionally, theoretical scanning tunneling microscopy has been performed over all the obtained structures in order to compare the results with those existing in previous literature, with a good agreement between experiments and theory. Particularly, all three adlayered configurations were found to form structures differing less than 1% in angles and lattice parameters with the experimentally detected structures [2].

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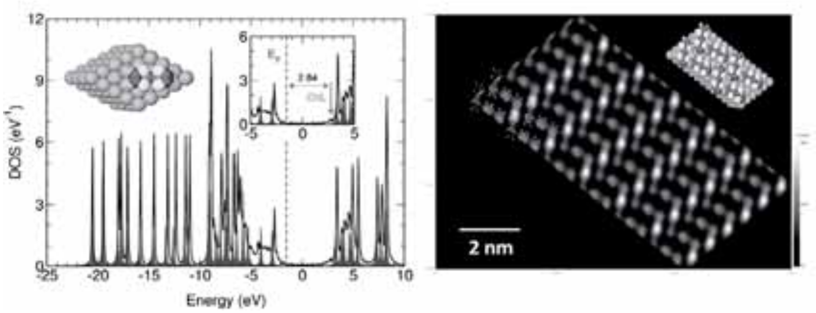

Image 1: Corrected PDOS of a single TTF molecule on Au(111), and theoretical STM of the TTF adlayered structure on Au(111).

Oxide nuclei propagation through the channel separating two dimer rows onto silicon(100) surface

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Previously, we have studied by using both first principles calculations and experiments the incorporation and the migration of oxygen molecules in the topmost layer of the Si (100) p(2x1) surface. The experimental results have been conducted to shed light into medium to low oxygen coverage oxidation. The first principles calculations have been performed to interpret these experimental results concerning the oxide nucleation, i.e. molecular oxygen dissociation and further incorporation of oxygen atoms into the silicon surface. We demonstrated that the incorporation of the first oxygen molecule leads to an oxide nucleus which corresponds to a silanone structure who takes place on a dimer unit of the surface without distortion of the silicon surface network.

Subsequently, the incorporation of a second oxygen molecule onto the dimer row exhibits drastic changes of the surface atomic arrangement that resulting oxide nucleus covers two adjacent dimer units. During this incorporation the silicon bonding arrangement is modified in the vicinity of the silanone that makes it possible to position an inter dimer oxygen bridging site [1]. The Si-O-Si created network is shown to draw a stable semihexagonal oxide pattern which offers a reasonable transition between the silicon cubic network and an amorphous oxide.

But the incorporation and the migration of oxygen atoms into the channel row is still open. STM experimental evidence suggests that the oxide nuclei can propagate through the channel separating two dimer rows. The question is here to understand how oxygen atoms incorporate and, as in the case of the dimer row, to which extent the channel is distorted. We will therefore present new results on the extension of the semi-hexagonal pattern along the surface with a specific attention on the oxide propagation through the silicon surface channel.

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Molecule-substrate interactions of ordered surface structures

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By utilizing concepts of supramolecular chemistry, increasingly complex self-assemblies with programmed architectures have been realized. The detailed structures and long-range order of such assemblies are governed by the balance between intermolecular and molecule-substrate interactions, the reversibility or irreversibility of intermolecular bond formation and the resulting availability or non-availability of structural repair mechanisms. In this work information on molecule-substrate interactions for the two perylene derivatives TAPP and DPDI adsorbed on Cu(111) is gained by combining experimental and theoretical studies.

TAPP/Cu(111) forms a porous network stabilized by the coordination of Cu-adatoms to the organic molecules through the lone-pairs of their nitrogen atoms. [1] By comparing experiment and theory, these adatoms are identified and the interaction between molecules, adatoms and the underlying substrate is analyzed, in particular with respect to the stability of the network and the specific commensurate geometry the molecules adopt on the Cu(111) surface. [2] For the second system, a porous network formed by DPDI on Cu(111), the influence of the network as a long-range-ordered periodic structure on the substrate is studied by scanning tunneling spectroscopy (STS) and angle-resolved photoemission spectroscopy (ARPES). In analogy to the band structure of a solid created by the periodic potential of its atoms it is in this case the periodic perturbation of the otherwise free-electron-like surface state that induces the formation of a weakly dispersive electronic band. [3]

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29 SEPT. | 15:00 | Poster Session

Ab initio studies of propene epoxidation at noble metal nanocatalysts

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Nanometer-sized gold particles have been reported as promising catalysts for the direct propene epoxidation reaction. Motivated by these results, recent experiments by S. Vajda and collaborators have studied the activity for this reaction of alumina-supported gold and silver nanocatalysts. In the case of gold, a remarkable activity and selectivity towards propene oxide formation is found for small sub-nm clusters (Au7-Au10). Silver nanoparticles (9-23 nm diameter) are also found active for propene oxide production, with the selectivity being strongly dependent on particle size and reaction temperature. In parallel to the experiments, ab-initio DFT simulations were performed to study both the stability of key reaction intermediates and the energy barriers for either acrolein or propene oxide formation. In the case of gold, the simulations confirm the superior catalytic activity of the small sub-nm clusters, and also a key role of thealumina surface oxygen anions during the formation of reaction intermediates. In the case of silver nanoparticles, the size- and corresponding morphology dependent theoretical activity and selectivity are in good accord with experimental observations: the edge sites that are more abundant in smaller particles enhance selectivity towards acrolein, whereas nanoparticle facet sites, which dominate for larger particles, preferentially form propene oxide.

Permanent magnetism in phosphine- and chlorine-capped gold clusters and nanoparticles

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Recent experimental results regarding the magnetic character of thiol-capped gold nanoparticles with element specific techniques (X-ray magnetic circular dichroism, XMCD, and Mössbauer spectroscopy) [1,2] have shown that magnetism is bounded to the gold surface atoms bonded to the thiol-protecting ligands. The research work presented here concerns the detailed study of the magnetic behaviour measured in phosphine-chlorine-capped gold nanoparticles (with core diameters around 2 nm). The investigation has been extended to subnanometric phosphine-chlorine-capped undecagold clusters. Both systems were synthesized in-house following a chemical route [3,4].

Transmission electron microscopy (TEM), scanning electron microscopy (SEM), X-ray absorption spectroscopy (XAS) and superconducting quantum interference device magnetometry (SQUID), have been used to discern the necessary conditions that give raise to a permanent magnetic moment. In addition, electron paramagnetic resonance measurements are used to rule out contributions to the magnetic moment from eventual ferromagnetic impurities. These experimental results reinforce the conclusions drawn from the previous works: the magnetic moment is located in the surface gold atoms. Additionally, when the NPs size decreases to the subnanometric size range the permanent magnetism disappears. The near edge structure of the XAS data, points out that charge transfer between gold and the capping system occurs in both cases. These results strongly suggest that nearly metallic Au bonds are also required for the induction of magnetic response.

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Rare Earth /gold surface compounds

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The high temperature reactive deposition of rare earths (RE) on Au(111) has been thoroughly investigated combining STM and Angle Resolved Photoemission (ARPES) experiments. These materials are attractive for their possible exploitation in several fields as magnetic recording or hydrogen storage. We have focused on the reactive epitaxy of Gd, La, and Ce, where we have found that, under specific growth parameters, one can obtain RE/Au alloyed monolayers and bilayers with extraordinary crystalline perfection. In the three investigated compounds, the optimum surface structure, namely the one exhibiting homogeneous alloying over the whole surface, corresponds to the REAu2 stoichiometry. Moreover, the lattice mismatch between the REAu2 layers and the Au(111) substrate gives rise to long-range periodic Moiré patterns, whose lattice constant vary from 32 Å in La to 33 Å in Ce and to 38 Å in Gd.

By means of ARPES we have studied the two-dimensional band structure of such surface alloys. The band structure is similar in all cases with minor spectral intensity and energy variations. The results have been compared with band structure calculations performed by M. Verstraete and A. Rubio within the European Theoretical Spectroscopy Facility (ETSF) project. Theoretical calculations and experimental bands basically agree to explain the band dispersion, energy position, and orbital nature of the bands. Fine variations among the different RE compounds are explained in qualitative terms.

Poster Session | 15:00 | 29 SEPT.

Surface states and structural stability in step lattices investigated with curved crystals

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Vicinal surfaces with periodic arrays of steps are attractive playgrounds for testing the fundamental properties of electrons in one-dimensional (1D) superlattices. In particular noble metals that feature the Shockley surface state. In a vicinal surface, the latter becomes a 1D superlattice state, and the step array exhibits structural instabilities at a terrace size *d* that matches the surface state Fermi wavelength $l_F/2$ [1,2]. By combining Angle Resolved Photoemission (ARPES) and Scanning Tunneling Microscopy (STM) we study, as a function of *d*, the evolution of Shockley electronic states and the lattice structure in step arrays using Au, Cu, and Ag curved crystals. In particular, around the 1D Fermi surface nesting points at which a structural/electronic interplay is expected.

Superlattice bands were obtained by ARPES across the three curved crystals. The band bottom energy allowed us to determine the d-dependent size effect that arises due to surface electron scattering and confinement within terraces. From the size effect, and using a simple Kronig-Penney model, we determine the scattering potential U_0b at step edges. We observe that U_0b increases from Ag, to Cu and to Au, but, surprisingly, it remains constant as a function of d in each crystal. The relatively large U_0b strength found in Au and Cu may explain the structural instabilities observed around Fermi surface nesting with $d=l_F$ and $d=l_F/2$. In Au the critical $d=l_F$ point coincides with the spontaneous faceting transition of Au(111) surfaces. In Cu, a strong change in terrace size broadening is observed between $d=l_F$ and $d=l_F/2$. In contrast, Ag surfaces do not apparently exhibit structural instabilities, which could indeed be explained as due to an insufficient electronic energy variation around $d=l_F/2$.

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Surface defects activate new reaction paths: formate formation during methanol decomposition on Ru(0001)

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We have carried out experiments of methanol adsorbed on Ru(0001) at room temperature during continuous gas exposure on surfaces with a variable density of defects. Surface defects were produced by high temperature annealing and controlled low energy ion bombardment. Surfaces and reaction products have been characterised by a combination of Auger Electron Spectroscopy (AES), Low Energy Electron Diffraction (LEED) and Infrared Reflection-Absorption Spectroscopy (IRRAS). We have identified novel reaction paths in the methanol/Ru(0001) system, mainly those leading to the complete or partial de-hidrogenation of the molecule. We show that a new reaction path appears just on the defective surface: the formation of formate (HCOO), which we identify for the first time during methanol adsorption on a metal. We propose that the presence of the defects (mainly steps) catalyzes the oxidation of formaldehyde to formate. This particular case shows how surface defects affect profoundly the catalytic activity, activating new reaction paths which are not available when the density of defects is low. We have also shown that reaction kinetics depend on whether the surface is flat or defective. Methanol dehydrogenation towards carbon monoxide proceeds at a higher rate in the presence of defects. Furthermore, intermediate products, namely methoxy (CH_3O), formaldehyde (CH_2O) and formyl (CHO) are stabilized by the increasing presence of CHx species, which in turn originate from methanol decomposition.

Study of surface chemical reactions induced by molecules electronically excited in the gas phase

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In a new experimental approach[1], based on application of total internal reflection phenomenon on an insulator surface, we localize laser photoexcitation in a narrow boundary gas layer just above the interface. Majority of the excited molecules can reach the surface before the relaxation. Approaching the surface, the electronically excited molecules will naturally experience strong acceleration and alignment. The energy of the excitation is likely to be converted to kinetic motion along the reaction coordinate for chemical adsorption. While recombination chemical reactions in a gas phase require participation of a third body, this strong limitation on the reaction rates is removed upon interaction with a surface.

The experiments are performed at high gas pressures, so that dense fluxes of the excited reagents can be readily produced. Products of chemical adsorption and/or chemical reactions induced within adsorbates are aggregated on the surface and observed by light scattering. Results of evanescent wave illumination are compared with those for laser beam propagating through the interface. We will demonstrate how pressure and spectral dependencies of the chemical outcomes, polarization of the light and interference of two laser beams inducing the reaction can be used to distinguish the new process we aim to investigate from chemical reactions induced by photoexcitation within adsorbed molecules and/or gas phase photolysis. High quantum yields for photochemical transformations are observed for some chemical substances (NO, SO_2). The experimental results may indicate an opening for investigations of a new, previously unexplored domain in photochemistry. The phenomenon observed and the experimental technique developed may have important perspectives for technological applications.

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Yeast Cytochrome C adsorption on gold substrates: a spectroscopic ellipsometry investigation

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Adsorption of Yeast Cytochrome C (YCC) on gold substrates has been studied with Spectroscopic Ellipsometry (SE). YCC is a relatively small protein belonging to the class of Heme-proteins which plays a key role in electron transfer between two membrane-bound enzyme complexes, through a reversible Fe (III) « Fe (II) process. We applied methods already successfully tested to study the growth dynamics of alkanethiols and other thiolate SAMS on gold [1-3]. In practice we have considered differences between spectra taken after and before the molecular layer formation ($\delta\Psi$ and $\delta\Delta$ patterns) in order to put SAM's spectral features in greater evidence. The SE investigation was carried out in situ in aqueous solution, at room temperature during protein deposition. Ex situ measurements on dried samples are also presented. SE data demonstrated the formation of a quite dense monolayer of YCC molecules, about 3-4 nm thick, in good agreement with molecular dynamics simulations of ref. [4] and consistent with Atomic Force Microscopy inspection. Both ex-situ and specially in situ difference spectra clearly show the YCC's Heme-related transition at 410 nm (the so-called Soret band), the same position found for the molecule in its buffer. Simulations of data have shown that the $\delta\Psi$ and $\delta\Delta$ difference spectra needs also a contribution from the transparent part of the molecule (Cauchy-type layer model) as already observed in another related protein SAM [5]. Analysis of the fine position of this Soret band allowed to obtain information on the oxidation state of the iron ion of the heme group, suggesting that the molecules have preserved their native structure.

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Strain-Spin Phase Diagram of Defective Graphene

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We present first-principles calculations of defective graphene under isotropic strain. We focus on the strain dependence of the properties of carbon monovacancies, with special attention in the spin moment. At zero strain the vacancy shows a spin moment of 1.5 Bohrs that increases up to 2 Bohrs with stretching. Changes are more dramatic under compression: the vacancy becomes non-magnetic under a compression larger than 2%. This transition is linked to the structural modifications associated with the formation of ripples[2] in the graphene layer. Our results suggest that defect-induced magnetism in graphene can be controlled using strain and other mechanical deformations[1].

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Adsorption of tetrathifulvalene (TTF) on Cu (100) at low coverages

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The study of molecular-inorganic interfaces is gaining increasing interest due to their large potential applicability to last generation electronic devices. In this sense, adsorption of organic molecules or layers on surfaces can combine a large variety of desirable properties, like conductivity, flexibility or cheapness of materials.

In this work, using Density Functional Theory methods, we have studied the adsorption of the organic tetrathiafulvalene (TTF) molecule on the Cu(100) surface at low coverages, where the available data seem to show a different adsorption geometry for the monomer (planar), as compared to the dimmer, trimer and tetramer case (vertical). We have analyzed in detail the interaction between the adsorbed TTF molecules and underlaying Cu(100) substrate considering different supercell configurations, chosen by two different criteria, i.e., the size of the supercell and the relative angle among the organic molecule and the surface. Our results indicate that, although the planar geometry is energetically favourable for TTF monomers, there is a weak attractive interaction between vertically adsorbed TTF dimers and, therefore, explains the observed tendency in STM topographical images.

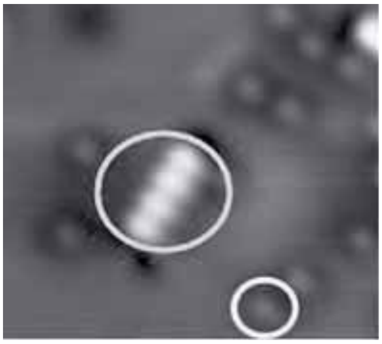

Figure: Experimental STM topographical image (courtesy from Amadeo L. Vazquez de Parga) taken in Ultra High Vacuum at 4.6 K at after room temperature deposition. The tunnelling conditios were V = - 1 Volt and I = 50 pA. The blue circle marks the location of a TTF tetramer, while the yellow that of a monomer. The brighter signal on the tetramer as compared to the weak one on the monomer reveals the difference in adsorption geometry: vertical (canted) for the tetramer and planar for the monomer.

Acknowledgements

We thank both MICINN (grant no. FIS2007-066711-CO2-01) and Gobierno Vasco – UPV/EHU (grant no. IT-366-07) for financial support and Amadeo L. Vazquez de Parga for permission to show their unpublished data.

Superlattice bands in tunable dislocation networks: structural/electronic interplay

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Moiré and strain dislocation networks arise when a monolayer or two of one material grows on a substrate with the same crystal symmetry but different atomic lattice constant. Beyond their use as growth templates, such metallic superlattices may be used as model two-dimensional metallic superstructures at which surface states scatter, thereby leading to two-dimensional superlattice band folding and gap opening. The Ag monolayer on Cu(111) system, with its characteristic free-electron-like surface state, is a prototype scenario. At low temperature, it forms a perfect coincidence lattice (Moiré), which transforms into a hexagonal array of triangular dislocations by annealing above 300 K. Such structural transition is accompanied by a deep surface state transformation, i.e., from a parabolic band in the Moiré structure to a superlattice-folded and gapped two-dimensional band structure in the dislocation network [1]. The latter features a full 25 meV gap that can be brought below E_F by lowering the temperature or by doping, thereby making the noble metal surface effectively semiconducting. On the other hand, it exhibits signatures of the nesting of the surface state Fermi surface by superlattice reciprocal vectors, strongly suggesting the presence of a charge-density-wave like state.

We have further investigated dislocation networks on noble metal overlayer systems. On the one hand, the alloyed Au_xNi_{1-x}/Ni(111) monolayer system, on which the superlattice periodicity varies as a function the stoichiometry *x* of the surface alloy. On the other hand, the Ag/Cu(111) system doped with minute amounts of K and Au atoms. In both cases, the superlattice band structure is observed to smoothly evolve with surface composition. Moreover, the latter can be tuned to force Fermi surface nesting, which in turn provokes lattice instabilities. We will discuss the connection between both, as well as give an estimate for the electronic/elastic energy inbalance in each case.

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29 SEPT. | 15:00 | Poster Session

Scattering of Vibrationally Excited H_2 from Metal Surfaces at Grazing Incidence

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Collisions of fast atoms with surfaces at grazing incidence have been proposed as a promising new tool to determine surface parameters with unprecedented accuracy [1-4]. Recently [5] we have shown, by means of classical dynamics calculations performed with first-principle six-dimensional potential energy surfaces that, under grazing incidence conditions, fast light molecular projectiles are also useful to determine sticking probabilities at thermal energies, from the threshold up to the saturation limit. Thus they are ideal complement to traditional experiments at thermal energies to determine sticking curves up the saturation limits. This striking result have been proved to be true for molecules in their ground rovibrational states and vibrationally excited in low v values. Very recently [6] it has been shown that dissociative adsorption probabilities curve, as a function of the incidence energy, for activated system present a nonmonotonic behavior for vibrationally excited molecules. This nonmonotonic behavior, observed whenever the vibrational energy is higher that the minimum reaction barrier, has been attributed to an inefficient reorientation of the molecule at low-medium incidence energies. The question we have address in the present work is: Can the nonmonotonic behavior for dissociative adsorption of $H_2(v>1)$ be observed under grazing incidence conditions? We will show how the answer to this question has been found to be positive.

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Hyperthermal Ar interactions with bare and adsorbate-covered Ru(0001) surfaces

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The study of gas-surface interaction dynamics is important not only for the fundamental knowledge it provides but also to aid the development of applications involving processes such as sputtering, plasma etching and heterogeneous catalysis. In this study, Ar atoms with hyperthermal energy (~6.3 eV) were scattered from bare, D-covered and CO-covered Ru(0001).

Hyperthermal Ar atoms were generated using a cascaded arc plasma source. Scattered Ar was atoms were detected by a rotatable, differentially-pumped mass spectrometer. Angularly-resolved intensity and energy distributions are derived from time-of-flight spectrometry. It is well known that atoms with hyperthermal energy may show structure scattering. However, Ar with 6.6 eV scattering from the Ag(111) surface shows a broad angular intensity distribution (hiding any structure scattering) and an energy distribution that tracks the binary collision model. The results from Ru(0001) show large differences as compared with those from Ag(111). The angular and energy distributions from Ru(0001) are consistent with scattering from a corrugated static surface. In addition, the results from the D-covered surface indicate that rainbow scattering occurs, confirming the presence of structure scattering. The differences between the results from bare and D-covered Ru(0001) are interpreted in terms of the stiffness of the surface.

Impinging Ar loses more energy at the CO-covered surface, to be expected due to the low CO mass. In addition, Ar collision-induced desorption of CO occurs leading to fast CO. The angularly-resolved CO desorption intensity distribution has a peak along the surface normal. This suggests that CO desorption process involves lateral interaction with neighbouring CO molecules.

29 SEPT. | 15:00 | Poster Session

Self-assembly of oligothiophenes functionalised with nucleosides

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Oligo- and polythiophenes are among the best investigated and most frequently used materials for optoelectronic applications, such as light emitting diodes or solar cells. Since polythiophenes often produce amorphous or semi-crystalline materials with little control over the material order, their oligomeric analogues moved more and more into focus of research. Due to their precise chemical structure, oligothiophenes give rise to well-defined functional properties, crystalline assemblies and discrete structure-property relationships.

During the past decade, the supramolecular assembly of oligothiophenes has been demonstrated as a promising approach towards improvement of device performances and big efforts have been made to direct the arrangement of the molecules. This is a still challenging task, because of the manifold of intermolecular interactions (e.g. van der Waals, p-p stacking and hydrogen bonding) which direct the molecular order and therefore influence the material properties.

Hence, the combination of semiconducting oligomers with well-understood self-assembling biomotifs might probably ease the rational design of novel nanostructured materials with interesting electronic properties. The combination of p-conjugated oligomers with nucleosides provides a versatile tool for non-covalent assemblies, taking advantage of the molecular recognition of the DNA base pairs [1]. In this work, the self-assembling behaviour of 1:1, 1:0 and 0:1 mixtures of conjugates desoxiadenosine$_2$-quaterthiophene (**A_2-4T**)and thymidine$_2$-quaterthiophene (**T_2-4T**) on highly oriented pyrolytic graphite (HOPG) was investigated by means of tapping-mode Atomic Force Microscopy (AFM). The conjugates comprise highly amphiphilic character and can exert various com–peting intermolecular forces. The images showed the formation of unconventional helix- and zigzag-like features (Fig. 1). In combination to spectroscopy measurements and semi-empirical calculations, a coherent picture that models the observed structures is given

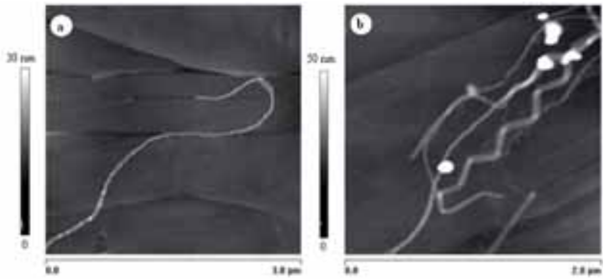

Fig. 1: AFM height images of a 1:1 mixture of conjugates **T_2-4T** and **A_2-4T.** Drop-casted on HOPG.

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Maximizing the magnetic anisotropy of ordered island arrays grown by self-assembly on Au(11,12,12)

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The main challenge of magnetic information storage is to increase the bit density without running into the super-paramagnetic limit where the magnetization reverses by thermal excitation. Industry investigates lithographically patterned media where one bit is one magnetic island. The bottom up approach by physical vapor deposition on template surfaces used here has the advantage to provide much smaller sizes and larger densities such that the ultimate limits of magnetic information storage may be explored. The key issues are to maximize magnetic anisotropy, minimize dipolar interactions, and to optimize uniformity of magnetic moments, easy axes, and switching fields.

Our template surface is Au(11, 12, 12), a vicinal surface enabling the growth of 5 x 7 nm spaced islands. Pure Co islands on Au(788) have been demonstrated to be uniaxial out-of-plane magnetized, to have narrow anisotropy distribution, and negligible dipolar interactions; the only drawback has been their relatively low blocking temperature of T_b = 50 K [1].

Therefore one of the figures of merit is the ratio between island size in atoms and blocking temperature. This number has to be small. For pure Co the record is 600 atoms for T_b = 85 K [2, 3], amounting to 7.1. We show here that Fe-shell Co-core islands with only 490 atoms have T_b = 105 K corresponding to a 40 % increase and a figure of merit of 4.7 [3]. The large anisotropy per atom can be rationalized by comparing with Co_xFe_{1-x} monolayers on Pt(111) [4].

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29 SEPT. | 15:00 | Poster Session

Dependence of thermal CO diffusion on local coverage

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The diffusion of adsorbates on surfaces plays a major role in many surface processes e.g. growth or reactions. In order to investigate the diffusion of single molecules, we deposited CO on Cu(111) at 22K. For analysis of the dynamics we then recorded several image series in the temperature range of 40K to 60K with a low-temperature scanning tunneling microscope. The diffusion of single CO molecules at low local coverages follows an Arrhenius law. At higher local coverages next-neighbor interactions influence the diffusion by modulating the local diffusion rates. We will discuss quantitatively the dependence of the diffusivity of single CO molecules on their local environment.

PASSION FOR
SOFT MATTER

ABSTRACTS

Soft Matter and Life Sciences: Research with Neutrons

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Research in soft matter deals with the integration of disciplines and subjects relating to objects such as colloids or polymers or amphiphilic molecules including living and synthetic matter. In this field a joint approach of disciplines like physics, chemistry, biology and simulation science are essential to arrive at novel insights. Challenges are e.g. the understanding (i) of selfassembly as the basic structuring mechanism in soft materials, slow and often hierarchical dynamics in complex environments, (ii) of out of equilibrium systems and (iv) the establishment of a bridge to biology. A molecular understanding of the associated phenomena require knowledge on the molecular structure and dynamics, that is revealed uniquely by scattering techniques and in particular the space time resolving neutron probe.

In my lecture I will go through results addressing the key challenges in the field. I will discuss the efficiency boosting effect by amphiphilic blockcopolymers in selfassembling microemulsions, I will present kinetic results on the structure formation in the selfassembly of polymer micelles. The dynamics of polymers in nanocomposites will serve as an example for the slow dynamics in complex environments and finally I discuss neutron spin echo experiments on the interdomain motions in alcohol dehydrogenase that are important in promoting biochemical function. There, neutrons reveal the domain displacement patterns and directly display the cleft opening dynamics between the binding and catalytic domains of this molecule that enable the binding and release of the functional important cofactor.

How anomalous remain the liquid water properties when confined at the nanoscale?

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The behavior of fluids confined within nanometric pores (size of a few molecular diameters) significantly differs from that of the bulk. The effect of confinement, surface forces, and reduced dimension is to shift the phase transitions of the confined fluid (condensation, freezing and crystallisation). By postponing or avoiding the inconvenient crystallization process it is often suggested that confinement allows a deeper penetration into the supercooled regime and could help in the understanding the glass formation. Confining liquid water at this scale is of special interest, since no experiments can be carried out below 240K in the bulk liquid state while this T-range, so-called ‘no-man’s land’, can be explored under confinement. However water and H-bonded liquids are perturbed by the presence of a surface which can modify its hydrogen bonding network and thus its energy, entropy and phase transformations. Thus a question always remains whether the confined liquid water -or any other fluid- is an extension of the “bulk” supercooled regime or refers to specific behavior controlled by external parameters such as the new length and the surface interactions imposed to the system. Despite the obvious fundamental interest in understanding bulk water, this situation corresponds to most of the cases in biological and geological systems and deserves particular attention per se. Here are presented new experimental results on the thermodynamic, structural and vibrational properties of water confined within nanometric pores (size of a few molecular diameters) in parallel to other H-bonded or van der Waals liquids.

Structure - dynamics relationship in nano-structured diblock-copolymers by dielectric spectroscopy

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Broad-band dielectric spectroscopy (BDS) is one of the most powerful methods to study the molecular dynamics under different sample environments, covering a huge frequency range (10^{-5}–10^{12}Hz). On the other hand, it is well established that the molecular dynamics of glass-forming systems in the range of the glass transition temperature is very sensitive to changes of control variables as temperature, pressure, concentration, etc. This is responsible for the strong changes in the dielectric relaxation behaviour in mixtures and crystallizing polymers as two typical representative examples. For instance, this sensitivity has allowed accessing the spatial scale characteristic of the polymer glass transition from the study of the component segmental dynamics of polymer-based mixtures.[1]

In this talk, the results obtained during the last few years from BDS experiments on several nano-structured diblock-copolymers will be presented. On one hand, the results on the micellar structure of polyisoprene (PI) -polydimethylsiloxane (PDMS) diblock copolymers with varying core size will be considered. From the dielectric relaxation originated by the (minority) PI segmental dynamics the concentration profile at the micelle interface was extracted[.2] The results agree well with those expected by the fluctuations of the interface induced by the presence of the high mobility PDMS chains in the surrounding. On the other hand, the PDMS nano-phase of strongly segregated diblock compolymers with polystyrene (PS) has been characterized. In this case, stiff PS limits the PDMS regions of high mobility, which produce an anchorage effect clearly detectable in the dielectric response.[3] Moreover, there are clear indications of a mobility gradient from the PS walls towards the PDMS core. Furthermore, in some cases, on cooling the PDMS regions embedded in the PS matrix cannot reach the PDMS melt density giving rise to a dramatic modification of the molecular motions in the PDMS nano-phase.[4]

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Water near proteins and under confinement: is that a good model for bulk water?

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The structural and dynamical properties of water confined in MCM-41-S and at the interface with globular protein lysozyme have been studied by Neutron Diffraction and Broadband Dielectric spectroscopy. The rationale behind these studies is manifold. In particular, it has been shown that hydration water plays an important role for enzymatic reaction, on one side, and the possibility to observe unfreezable confined water well below 235 K, opens to interesting comparison with the properties of bulk water.

The dynamics of the hydrogen bond network of a percolating layer of water molecules adsorbed on lysozyme has been looked at by measuring the temperature dependence of the relaxation time of water protons.
We observe two dynamic crossovers: (i) at T~252 K, which we assign to water proton fluctuations along the growing hydrogen bond network; (ii) at T~181 K which we interpret as arising from a structural ordering of the water network. We support this interpretation by comparing our experimental results with calculations on a cell model of water, showing that the two crossovers correspond to two maxima in the specific heat, each associated with a structural change of the hydrogen bond network: the formation of the network at higher T, and its ordering at lower T. Interestingly, the results obtained with the cell water model do not depend on the dimensionality of the system, and as such could be relevant to bulk water as well.

The structure of confined water has been looked at by performing neutron diffraction experiments with isotopic substitution. It is fair to say that water's behavior under confinement is incompletely understood. These depend on the properties of the confining surfaces, although a number of characteristics common to all confined waters, such as non uniform volume occupancy and depression of the ice nucleation temperature, may still be identified. Here we show that, even at fixed confining substrate characteristics, confined water cannot be considered a single well defined system, and several water-like structures can be identified within the same volume at the same temperature.

These experimental findings suggest conflicting answers to the question on the similarities between bulk and confined water, and reveal other puzzling characteristics of the most complex liquid (un)known.

Confined Water | 12:20 | 28 SEPT.

Designing ion-containing polymers for facile ion transport

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We synthesize single-ion conducting ionomers with low glass transition temperatures to prepare ion conducting membranes for actuators and lithium battery separators. We use dielectric spectroscopy to determine the number density of conducting ions and their mobility from electrode polarization (using the 1953 Macdonald model) and the number density of ion pairs from measured dielectric constant (using the 1936 Onsager model). This experimental work concludes that the number density of conducting ions is tiny, and we discuss ways to boost that using more polar polymers with weak-binding anions attached to the chain.

We use *ab initio* quantum chemical calculations at 0 K in vacuum to characterize ion interactions and ion solvation by various functional groups on ion-containing polymers. Simple ideas for estimating the ion interactions and solvation at practical temperatures and dielectric constants are presented that indicate the rank ordering observed at 0 K in vacuum should be preserved. Hence, such *ab initio* calculations are useful for screening the plethora of combinations of polymer-ion, counterion and polar functional groups, to decide which are worthy of synthesis for new ionomers. The results provide estimates of parameters for a simple four-state model for counterions in ion-containing polymers: free ions, isolated ion pairs, triple ions and quadrupoles. We show some examples of how ab initio calculations can be used to understand experimental observations of dielectric constant, glass transition temperature and conductivity of polymerized ionic liquids with either lithium or ionic liquid counterions.

Thermodynamic and Kinetic Models of the Appearance of Biological Chirality

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Chiral asymmetry choices exhibited by molecules that are present in living organisms constitute a scientifically challenging set of observations. Such geometric preferences favoring one enantiomer over its mirror image are obvious in the observed structures of amino acids, sugars, and the biopolymers that they form. These facts automatically generate fundamental questions about how those chiral asymmetries arose spontaneously in the terrestrial biosphere [1, 2].

We have formulated thermodynamic [3] and kinetic [4] models of chiral amplification. In the thermodynamic case, we model the phase behavior of a ternary mixture composed of two enantiomeric forms of a chiral molecule and a non-chiral liquid solvent. The mean-field solution of the model allows the calculation of a ternary phase diagram, a prominent feature of which is the existence of two symmetric triple points involving coexistence of a liquid phase enriched in one of the enantiomers, a racemic crystal, and an enantiopure crystal. Over broad ranges of initial composition, including liquid mixtures containing almost equal amounts of the two enantiomers, thermodynamic equilibrium results in liquid-phase chiral amplification, in agreement with experimental observations [5].

The kinetic model involves an auto-catalytic reaction leading to the formation of a chiral compound, inhibition, and molecular diffusion. Numerical solution of the model via kinetic Monte Carlo allows the identification of two types of behavior. In one, the system evolves towards a mixture containing equal amounts of the two chiral enantiomers. In the symmetry-broken regime, the system evolves spontaneously towards large excess of one or the other chiral enantiomers. We map the regions of parameter space leading to symmetry breaking.

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Emerging Properties | 09:50 | 29 SEPT.

Dynamic Asymmetry Effects on Self-assembly: Neutron is a Marvelous Probe to See Their Rich Varieties Ranging from Viscous-to-Gel Limits.

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We review the experimental results and the theoretical analyses concerning the self-assembly of the multi-components systems with dynamic asymmetry, in which constituent molecules or structural elements have a large difference in mobility. The dynamically asymmetric systems, i.e., polymer solutions, polymer mixtures, colloid dispersions, gels, etc. (soft matters in general), the local mechanical stress, built up naturally during their structural evolutions, is sustained primarily by slowly-moving components, because the stress by faster moving components relax faster than the others. This stress imbalance and its relaxation strongly affects the self-assembly of dynamically asymmetric systems, through a dynamical coupling between stress and diffusion. The dynamic asymmetry has a rich variety in its effects ranging from the viscous limit to the gel limit; it gives profound effects on pattern formations via phase separation with or without external fields and on dynamics of the concentration fluctuations in a single-phase state.

In this paper, let us specially focus on a binary polymer mixture of polystyrene (PS) and poly (vinylmethylether) (PVME). In addition to a lower critical solution temperature (LCST) type phase diagram for its mixing behavior, the PS/PVME mixture has a large difference in the glass transition temperatures (T_g) for the consituent polymers ($T_{g,PS}$ = 383 K and $T_{g,PVME}$= 253 K). Because of the large difference in T_g, we are able to tune dynamic asymmetry (or a_a) by changing temperature.[1] At the same time, a crossover from the viscous limit to the gel limit occurs, when the mixture temperature crosses $T_{g,PS}$. Focusing on the intermediate temperature region between $T_{g,PS}$ and $T_{g,PVME}$, we discuss **the anomalous suppression of small-angle scattering in a quiescent state** [1,2, ref] originating from a gel limit. Related to the topics, **shear-induced phase separation** of the PS/PVME mixture was investigated by 3-dimensional small-angle neutron scattering (3d SANS). 3 VI-3. These findings will be discussed in a theoretical framework of the dynamical coupling between stress and diffusion, which was developed by Onuki and Doi.[4] A focusing neutron ultra-small-angle scattering method,[5] employing focusing neutron lenses plays a crucial role to clarify the intriguing effects appearing in the mesoscopic length scales. The concepts and experimental methods reviewed in the text will be applied to the self-assembly in chemical gels, 6 chemically reacting systems and even to a living cell.

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Stimuli-Responsive Block Copolymer Micelles and Gels in Ionic Liquids

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Block polymers provide a remarkably versatile platform for achieving desired nanostructures by self-assembly, with lengthscales varying from a few nanometers up to several hundred nanometers. Ionic liquids are an emerging class of solvents, with an appealing set of physical attributes. These include negligible vapor pressure, high chemical and thermal stability, tunable solvation properties, high ionic conductivity, and wide electrochemical windows. For various applications it will be necessary to solidify the ionic liquid into particular spatial arrangements, such as membranes or gels, or to partition the ionic liquid in coexisting phases, such as microemulsions and micelles. We have begun a systematic exploration of ways to achieve this by block copolymer self-assembly.

One example includes formation of spherical, cylindrical, and vesicular micelles by poly(butadiene-*b*-ethylene oxide) and poly(styrene-*b*-methylmethacrylate) in the common hydrophobic ionic liquids [BMI][PF6] and [EMI][TFSI]. This work has been extended to the formation of reversible micelle shuttles between ionic liquids and water, whereby entire micelles transfer from one phase to the other, reversibly, depending on temperature and solvent quality. Formation of ion gels has been achieved by self-assembly of poly(styrene-*b*-ethylene oxide-*b*-styrene) triblocks in ionic liquids, by the thermoreversible system poly(N-isopropylacrylamide-*b*-ethylene oxide-*b*-N-isopropylacrylamide), and by hydrogen bonding between poly(vinyl phenol) and poly(2-vinylpyridine-*b*-ethyl acrylate-*b*-2-vinylpyridine), using as little as 4% copolymer.

Morphological Transition Kinetics in Amphiphilic Block Copolymer Micelles Explored by Small-angle Scattering in the millisecond range

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The kinetic pathways of block copolymer micelle systems are still not understood. Earlier we have focussed on the formation kinetics where we showed that the kinetic pathway is characterised by a nucleation & growth type mechanism where unimer (single) chain is the dominating fundamental step [1]. Here we focus on the structural and kinetic aspects of a cylinder-to-sphere structural transition occurring in a model amphiphilic block copolymer system upon variation of the interfacial tension. We demonstrate that the transition is governed by entropic chain stretching in the core, which is more prominent at high interfacial tensions. We further show that we can directly follow these transitions in the real time by small angle scattering using both neutrons (TR-SANS, D11, ILL) and by x-rays (TR-SAXS, ID02, ESRF) by applying a stopped-flow apparatus for rapid mixing. The results show that the cylinders typically are broken into a mixture of dumbbell- and sphere-like structures within some few hundreds of milliseconds and thereafter reorganize to the final equilibrium spherical micelles within seconds. Interestingly the opposite transition is not possible where the system rather ends up in a into another spherical micellar state. We will discuss this behaviour in connection with some recent results on the respective “equilibrium” exchange kinetics that can be accessed using time resolved SANS [2]. We will try to interrelate and discuss the relation between equlilibrium and non-equilibrium kinetics in block copolymer micelles and how this insight might be used to create cost-effective nano-particles.

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Computer simulations of polymer blends: from structural relaxation to chain dynamics

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The widespread potential applications of polymer blends have spurred a great deal of recent research effort on the dynamics of these systems showing tunable properties. Thermodynamically miscible polymer blends exhibit complex dynamics. They show dynamic heterogeneity in the meaning that two different segmental relaxations can be observed in the blend state. When the two blend components exhibit very different segmental mobilities, and at low concentrations of the fast component, the latter is strongly restricted ("confined") by the slowly relaxing matrix formed by the slow component.

In this talk we present recent research by the Polymers and Soft Matter Group of San Sebastián on dynamically asymmetric polymer blends by means of computer simulations. We investigate models for polymer blends of differents complexities, from simple bead-spring systems to fully-atomistic force fields. The obtained results exhibit anomalous dynamic scenarios which seem to be generic for the fast component in polymer blends with strong dynamic asymmetry. Such unconventional features extend over a broad range of dynamic length and time scales, from the structural relaxation to the chain end-to-end reorientation, and include:

i) Extremely stretched, quasi-logarithmic relaxations of density correlators.
ii) Decoupling of dynamic collective correlations and self-motions.
iii) Unexpected analogies with the dynamics of entangled homopolymers, for the relaxation of the chain normal modes in *non-entangled* blends.

We discuss the features i) and ii) in the context of the Mode Coupling Theory of the glass transition, as the result of a competition between two mechanisms for dynamic arrest with distinct characteristic lengths: generic packing effects, and confinement induced by the slow matrix. The feature iii) suggests a more fundamental physical basis, beyond usual reptation-based models, for observations usually associated to entanglement effects. Possible connections with theoretical formalisms based on memory kernels are discussed.

The Structure of Protein-Surfactant Complexes from Small-Angle X-ray Scattering

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Protein-surfactant interactions have central roles in fundamental science, in many biotechnologies and in industrial processes in, e.g., the food industry, pharmaceutical industry, and, of course, in fabric and homecare detergent industry. For enzymes, the interaction with surfactants may lead to denaturing of the protein and loss of activity or it may stabilize the structure and enhance the activity. For proteins with a tendency to aggregate and form amyloid fibrils similar to those found in many neuro-degenerative disorders such as Parkinson’s, Creutzfeldt-Jakob’s and Alzheimer’s diseases, the addition of small amount of surfactants may inhibit or promote the formation of fibrils. With this variety of the influence of surfactants on different proteins, it is important to gain more detailed knowledge on specific protein-surfactant systems, and in particular on the structures formed. We have performed two studies in which we have obtained structural information by small-angle X-ray scattering in combination with spectroscopic and calorimetric techniques. In the first project we have investigated the binding of Sodium Dodecyl Sulphate (SDS) to the alpha-helix protein, acyl-coenzyme A-binding protein (ACBP) [1]. In this system, SDS leads to a gradual unfolding and denaturing of the globular ACBP molecule. SAXS has shown that at low SDS concentration, well below the critical micelle concentration, complexes are formed with a small SDS micelle associated with two ACBP molecules with part of the ACBP molecules protruding into the solvent. At higher concentration, the complexes have one ACBP per micelle tightly bound to the headgroup region of SDS on the surface of the micelles. In the second project, we have studied SDS-induced fibrillation of alpha-synuclein (aSN) by SAXS [2]. The surfactant induces secondary structure in aSN which is naturally unfolded. At low SDS concentration, SDS micelles associate as pearls on a string in highly disordered structures that grow as a function of time. For higher SDS concentration, stable complexes are formed that contain a decreasing number of micelles for increasing concentration of SDS. This has established a direct connection between thermodynamic and structural information by combining SAXS with isothermal titration calorimetry and other spectroscopic techniques. Our work provided an understanding of the molecular basis of surfactant-induced protein aggregation, and also clarified why exactly SDS gives a unique reproducible aggregation.

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28 SEPT. | 15:00 | Window to Biology

Directed Self-Assembly of Block Copolymers over Macroscopic Length Scales

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A novel process to prepare highly oriented and aligned arrays of block copolymer microdomains over macroscopic distances will be described. Ultra-high density dot patterns and line patterns have been produced on surfaces having textured with facets from a single crystalline material. These facets are very small in amplitude in comparison to the period of the block copolymer and the pitch of the facets do not need to commensurate with the period of the bock copolymer microdomain array. Both experimental and theoretical studies will be discussed outlining the manner in which the alignment and orientation occurs and the extension of this to soft surfaces and, potentially, roll-to-roll processes will be discussed. Characterization and quantification of the lateral ordering was done by transmission electron microscopy, scanning force microscopy, in situ small angle neutron and x-ray scattering and grazing incidence small angle x-ray scattering (GSAXS). Efforts to use GISAXS as a metrological tool for the characterization of the lateral ordering will be presented

Self Assembly of Janus Particles and other Patchy Colloids

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In the talk I will report novel numerical results on the behavior of primitive models of patchy particles with the aim of understanding the interplay between phase separation and self-assembly and how the fraction of surface allowing for attractive interactions controls the collective behavior of the system. The case of Janus particles, i.e. particles characterized by a surface divided evenly into two areas of different chemical composition, will be discussed in details. Finally, I will discuss how simple models of patchy particles can help clarifying the behavior of colloidal systems in which the "valence" is controlled by the temperature, as in the case of dipolar hard spheres.

Recent literature related to this presentation includes:

1] E. Bianchi, J. Largo, P. Tartaglia, E. Zaccarelli, F. Sciortino Phase diagram of patchy colloids: towards empty liquids Phys. Rev. Lett. 97, 168301, 2006
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3] F. Sciortino, E. Bianchi, J. Douglas and P. Tartaglia; Self-assembly of patchy particles into polymer chains: A parameter-free comparison between Wertheim theory and Monte Carlo simulation J. Chem. Phys.126, 194903, 2007
4] Francesco Sciortino, Cristiano De Michele, Silvia Corezzi, John Russo, Emanuela Zaccarelli and Piero Tartaglia
A parameter-free description of the kinetics of formation of loop-less branched structures and gels
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5] Francesco Sciortino, Achille Giacometti and Giorgio Pastore
Phase Diagram of Janus Particles, Phys. Rev. Lett. 103, 237801 (2009)
6] J. M. Tavares, P. I. C. Teixeira, M. M. Telo da Gama and F. Sciortino
Equilibrium self-assembly of colloids with distinct interaction sites: Thermodynamics, percolation, and cluster distribution functions J. Chem. Phys. 132, 234502 (2010).

29 SEPT. | 10:20 | Emerging Properties

Slow Dynamics in Soft Glassy Materials

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By combining and extending mode coupling, dynamic density functional, and stochastic nonlinear Langevin equation methods [1], microscopic theories for thermally activated glassy dynamics in dense fluids and suspensions of spherical and nonspherical particles, which can be hard or soft and repulsive or attractive, have been developed based on the unifying concept of a dynamic free energy. True solids emerge only as jamming is approached with a divergent relaxation time of an essential singularity form, and intermittent barrier hopping results in multiple dynamic heterogeneity effects [2]. Kinetic vitrification and the alpha relaxation time of repulsive uniaxial objects are nonmonotonic functions of aspect ratio, exhibit a re-entrancy behavior as attractive forces are introduced, and are characterized by a shear modulus that increases exponentially with volume fraction and obeys a universality based on a critical concentration [3]. These predictions are in good agreement with recent experiments on dense suspensions of dicolloids [4]. Coupled translation-rotation activated dynamics has also been studied based on a dynamic free energy surface [5]. A plastic glass state is predicted at low aspect ratios, and multi-dimensional Kramers theory allows a mechanistic understanding of cooperative hopping dynamics and fragility. Dense solutions of controllably soft repulsive particles, such as many arm stars and microgels, have also been studied [6]. For particles that interact via a Hertzian contact repulsion, the kinetic arrest diagram in the reduced temperature (or single particle stiffness) versus volume fraction plane shows no activated dynamics regime below a critical repulsion strength. When activated dynamics does occur, the relaxation time as a function of volume fraction increasingly resembles a strong glass former, and the shear modulus grows more weakly with concentration, as the particle becomes softer. At fixed volume fraction, an increase of particle stiffness results in a broad range of dynamic fragilities which partition into two qualitatively different categories that can be understood based on jamming and scaling concepts. Comparison of the theoretical results with recent experiments and simulations on soft particles reveals good agreement. The theoretical approach has also been generalized to treat relaxation, physical aging, and nonlinear mechanical response in cold polymer liquids and glasses [7]. This work was done in collaboration with Jian Yang, Rui Zhang, Erica Saltzman, Galina Yatsenko, Ryan Kramb and Chip Zukoski.

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Decoupling phenomena in dynamics of Soft Matter: From small molecules to proteins

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Traditional physical picture suggests that solvent friction ultimately defines molecular motions in a liquid (e.g. diffusion, rotation). The solvent friction is connected to the structural relaxation. Thus the traditional picture assumes that major relaxation processes in a liquid should be coupled and should exhibit the same temperature variations. Experimental studies, however, reveal strong decoupling in rotational and translational motions in molecular liquids, decoupling of global chain relaxation and more local segmental dynamics in polymers. We present an analysis of various decoupling phenomena, from small molecular liquids, to polymer melts and proteins in solutions. We demonstrate that the decoupling in dynamics of so different materials has a general behavior and is stronger in more fragile systems (systems with steeper temperature dependence of structural relaxation). We ascribe the decoupling phenomena to dynamic heterogeneities on the nanometer scale that affect significantly structural relaxation, but are averaged out on time- and length-scales of other processes (e.g. diffusion, chain dynamics, protein relaxation). At the end we discuss how the decoupling phenomena can be used in various applications from energy to bio- technologies.

30 SEPT. | 09:50 | Dynamic at Different scales

Pattern evolution - From viscoelastic phase separation to mechanical fracture

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Phase separation is one of the most fundamental phenomena that create spatially inhomogeneous patterns in materials and nature. It has so far been classified into three types: (i) solid, (ii) fluid, and (iii) viscoelastic phase separation. The relevant transport processes are only diffusion for (i), diffusion and hydrodynamic convection for (ii), and diffusion, hydrodynamic convection, and mechanical stress for (iii). Here we report another phase-separation behaviour accompanying fracture, which is observed under a sufficiently deep quench in polymer solutions. Surprisingly, fracture becomes a dominant coarsening process of the phase separation. Under a deep quench, a transient gel is formed by strong attractive interactions between polymers. The connectivity of the polymer network acts against phase separation and produces the internal stress field. When this stress field exceeds the mechanical stability limit of the transient gel, mechanical fracture takes place: fracture phase separation. The behaviour of viscoelastic and fracture phase separation originates from a strong coupling between composition and deformation field. We demonstrate that the same type of coupling between density and deformation field leads to cavitation of fluid under shear and mechanical fracture of glassy liquid and solid under deformation. The key common concept is "dynamic asymmetry". We discuss a common physics underlying these apparently unrelated phenomena and a selection principle of the kinetic pathway of pattern evolution. For example, the only difference between phase separation and fracture may stem from whether deformation is produced internally by phase separation itself or externally by loading.

Deviations from Chain Ideality in Polymer Melts

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A cornerstone of modern polymer physics is the “Flory ideality hypothesis”. This hypothesis states that polymer chains in a three-dimensional melt have random-walk-like conformations. However, recent theoretical and numerical results suggest that this view is an oversimplification. There are noticable deviations from chain ideality, resulting from the interplay of chain connectivity and the incompressibility of the melt. This interplay leads to a swelling of chain segments and thus to a perturbation of the postulated ideal chain conformation. The swelling manifests itself in several ways. For instance, the bond-bond correlation function of two bonds separated by a spatial distance r between the bonds displays a long-range power law decay, and there are wave-vector dependent deviations from the Kratky plateau for the form factor of a chain. We will present a brief overview of these results and then turn to the case of strictly two-dimensional polymer melts, where the chains adopt compact, segregated conformations with an irregular (fractal) chain contour. Using molecular-dynamics simulations and scaling arguments we discuss the conformational properties of the chains, in particular their form factor. We also briefly address the chain dynamics which is well described by a model where shape fluctuations occur in an amoeba-like fashion through the advancing and retracting of contour ``lobes´´. This leads to long-range spatio-temporal correlations of monomer displacements, as evidenced by the power-law behavior of the chains´ center-of-mass velocity auto-correlation function.

Dynamics in polymer nanocomposites

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Nanoparticles added to polymers can enhance mechanical, electrical and thermal properties. Moreover, the polymer processing conditions can be changed by the addition of NPs because molecular relaxation is perturbed by the filler. Using elastic recoil detection, we have found that the addition of single walled carbon nanotubes to a polystyrene matrix produces a minimum in the diffusion coefficient with increasing nanoparticle concentration. Initially, tracer diffusion coefficients are suppressed with increasing nanotube concentration and then increase beyond a critical concentration. Shorter tracer chains exhibit a greater slowing down than longer chains, whereas longer matrix chains decrease the value of the critical nanotube concentration. The experimental results are interpreted in terms of locally anisotropic diffusion perpendicular and parallel to the nanotube filler and simulated using a trap model that defines a trap size and the extent of slowing perpendicular to the cylindrical trap. The simulated diffusion coefficients capture both the initial decrease in the diffusion coefficient attributed to isolated traps and the recovery of the diffusion coefficient above the critical concentration corresponding to trap percolation.

For polymer tracer diffusion in multiwall carbon nanotube / polymer nanocomposites, we again find that the tracer diffusion of 680k deuterated polystyrene is strongly suppressed at low MWCNT concentrations and then increases at higher concentrations. In contrast, the tracer diffusion of 10k dPS and 75k dPS is independent of MWCNT loading. These results reveal an important criterion for exhibiting a minimum in the tracer diffusion coefficient with nanoparticle concentration, namely the relative size of tracer molecule and nanoparticle. Specifically, when the radius of gyration of the tracer polymer, R_g is smaller than the radius of the nanotube particle, R_{CNT}, the tracer diffusion is independent of nanoparticle concentration, while a minimum is observed when $R_g > R_{CNT}$.

Water and "The Others": Simulations of Supercooled Water in Confinement and Solutions.

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In the past years several theoretical and experimental studies have led to a picture according to which the anomalous properties of water might be due to the presence of a liquid-liquid phase transition in the supercooled region possibly terminating in a liquid-liquid critical point. On the other hand water also shows upon supercooling a behaviour typical of a glass former approaching the Mode Coupling Theory crossover temperature.

I will show molecular dynamics simulations results of deeply supercooled water confined in a cylindrical pore of MCM-41 silica material [1]. A fragile to strong (FS) dynamic transition at T=215 K is located analogous to what recently found in experiments on water in MCM-41 and in simulation of the bulk. The maximum found in the specific heat at the FS transition suggests that this transition is related to the crossing of the Widom line, indicating the presence a low density and high density liquid-liquid coexistence. I will also show a study of the phase diagram of water in the supercooled region of ionic aqueous solutions [2] and of Jagla water-like particles in solvophobic solutions [3] aimed to clarify the effect of these species on the liquid-liquid critical point phenomenon. In particular the positions of the liquid-liquid critical point in bulk water and in a c = 0.67 mol/kg solution of water in sodium chloride are located and the critical point in the solution appears in principle experimentally accessible.

All these studies point out that experiments on confined water and in solutions are extremely relevant for the comprehension of low temperature bulk properties, supporting the idea of a unified scenario for supercooled water encompassing dynamics and thermodynamics.

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28 SEPT. | 12:50 | Confined Water

Dynamic heterogeneity in binary poly(ethyl acrylate) /p-xylene mixtures

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The present work deals with the investigation of polymer dynamics in poly(ethyl acrylate, PEA)/p-xylene binary mixtures. PEA chains are either linear chains or in the form of networks with varied cross linking densities whereas p-xylene is a crystallisable non polar solvent. The aim of this study is to investigate the characteristics of dynamic heterogeneity in such mixtures where PEA networks with varied viscosities are swollen by the same non-polar solvent. Differential Scanning Calorimetry (DSC), Thermally Stimulated Depolarization Currents (TSDC) and Dielectric Relaxation Spectroscopy (DRS) were the experimental methods of investigation. Our results allow the construction of the so-called phase diagram for the binary mixtures. We are able to follow the PEA dynamics (both segmental and local chain motions) in homogeneous mixtures (at low solvent contents) and in systems with partial p-xylene crystallization (at high solvent contents) as well. The results are discussed in terms of chain mobility, shape and strength of the relaxation processes. The influence of p-xylene molecules (molecularly distributed or phase separated) on the molecular dynamics of the PEA network was systematically studied. Our results reveal that below a critical solvent concentration, c_{pxcrit}, (c_{pxcrit} depending on the PEA viscosity) the decrease of the T_g of the mixture as a function of the p-xylene content is well described by the Fox equation, indicating the homogeneous character of the mixing of the two components (plasticization action of p-xylene). For this c_{px} region the results imply that the mixtures are dynamically homogeneous. For $c_{px} > c_{pxcrit}$, a fraction of p-xylene crystallizes and the PEA/p-xylene mixtures exhibit a constant glass transition temperature corresponding to the gel phase of PEA with the non-freezable p-xylene fraction. In this c_{px} region the mixtures become dynamically heterogeneous. Interestingly, the unfreezable p-xylene content has been found to depend on the viscosity of PEA network implying that the amount of non-freezable solvent is mainly controlled by diffusion phenomena.

The dynamical behaviour of water confined in perfluorinated ionomers and surfactants.

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Perfluorinated ionomers, the reference membranes for fuel cells, are characterized by an hydrophobic/hydrophilic nanophase separation. Water is the medium for proton transfer: it plays a central role, although not yet fully elucidated, in the conduction mechanisms that need to be optimized for the ongoing development of new efficient fuel cells. The dynamical properties of the water are severely affected by the confinement in the charged matrix at the nanometric scale. The relaxation times associated to the proton diffusion range from the picosecond (local jump of a proton between two ionic groups) to few tenths of seconds (macroscopic conductivity through the whole membrane).

In order to clarify the structure-to-transport relationship in ionomers, we have studied by Quasi-elastic Neutron Scattering and Molecular Dynamics Simulations the behaviour of water in different systems: perfluorinated membranes (Nafion [1], aged Nafion, and short-chain Acquivion ion) and surfactants [2]. The latter mimic the physico-chemical properties of the real systems and offer the advantage to self-assemble in well defined organized phases.

The QENS study have been performed on both time-of-flight and backscattering spectrometers. The quasielastic spectra are discussed on the basis of a sophisticated model for confined motion: the Gaussian model [3]. This unique diffusion model based on Gaussian statistics takes into account both localized translational motions and long-range diffusion. Comparison of the diffusion mechanisms and parameters (diffusion coefficients, characteristic confinement sizes and relaxation times) obtained in the various systems as a function of their hydration bring new insight on the complex molecular scenario for proton motion under confinement.

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Electrostatics and viscoelasticity of protein-water interface

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Electrostatics and elasticity of the surface of hydrated proteins have been studied by numerical simulations. We found that the statistics of electrostatic potential fluctuations inside biopolymers are highly non-Gaussian, with a very broad breadth of fluctuations. This phenomenon disappears with lowering temperature at the point of dynamical transition in proteins when the linear response approximation starts to apply. The related change from non-harmonic to harmonic mean square displacement of protein atoms, seen in Moessbauer spectroscopy, is analysed by a viscoelastic dynamics of the protein-water interface. It is shown that the onset of anharmonic protein conformations is connected to the appearance of overdamped viscoelastic modes in the instrumental observation window. The non-Gaussianity of the electrostatic fluctuations is related to the formation of dynamical ferroelectric domains within the protein hydration layer. This property provides an order of magnitude increase in the energetic efficiency of enectron tranport chains in biology.

Study of Nanoscale Protein Dynamics by High Power Neutron Spectroscopy

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The intimate relation between functionality and molecular level dynamics in proteins is a widely accepted conjecture, although not without controversy. Experimental evidence has been provided by the observations of the close correlation between functional kinetics and various observed signatures of microscopic dynamics, such as the Lamb-Mossbauer factor. More recently the use of a combination of various spectroscopic tools, including dielectric relaxation and a host of inelastic neutron scattering techniques covering many orders of magnitude across the ps and ns time domain. Full blown spectroscopy opens up new opportunities to go beyond the natural limitations of indirect observations of dynamics, such as the Lamb-Mossbauer factors. The results allowed us to identify of a number of key features of the dynamic process associated with onset of protein functionality. These features show close analogy to the beta type of relaxation processes in glasses, spreading over an unconventionally broad time domain between microscopic and macroscopic times in a dynamically heterogeneous fashion.

Probing the multi-level structure and dynamics of soft matter using X-ray scattering

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This presentation will give an overview of different possibilities offered by synchrotron X-ray scattering techniques in the investigation of soft matter systems. Recent advances in synchrotron instrumentation and data analysis methods allow highly quantitative structural studies from nanometer to micron scale with millisecond time resolution [1]. The primary goal of such time-resolved experiments is to gain better insight into the kinetic processes and offer predictive capability. This will be illustrated by two examples, the self-assembly of amphiphilic molecules to form unilamellar vesicles and complexation of natively unfolded proteins such as casein micelles. In these investigations, probing the structural kinetics in turn provide a comprehensive understanding of the underlying nanostructure.

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Hidden Macroscopic Shear Elasticity in Viscous Liquids

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Liquids are defined by the absence of shear elasticity in contrast to solids or plastic fluids that require a finite stress to flow. But, what is the validity of this definition? Recent studies have shown that actually long-range elastic correlations have been *hitherto* neglected in the liquid state far away from any transition[1].

The solid-like nature of liquids revealed by examining the dynamic response of viscous liquids, glass formers, molten polymers is a finding of major importance. This non-vanishing macroscopic shear elasticity modifies the conventional understanding of the liquid state. The finite shear elasticity has to be taken into account to improve the analytical approach. It should shed light on numerous unpredictable phenomena (over large time scale relaxations, spectacular instabilities, spurt effect, supercooled effects, "shark-skin" instability), particularly visible in highly viscous liquids like glass-formers or polymeric melts. A special attention will be paid to polymer melts in the light of the viscoelastic approach and the formalisms of Rouse and reptation representative of the elementary molecular dynamics[3,4]. This single molecular picture neglects intermolecular interactions and thus ignores the cohesive nature of the fluidic state. The identification of finite shear elasticity points out the role of the intermolecular interactions in the dynamic properties and restores the cohesive character of the liquid missing in the viscoelastic approaches.

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Influence of pressure on fast relaxation in glass-forming materials

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The spectra of GHz-THz dynamics in glass forming materials have two main contributions: one is the boson peak and another is the fast relaxation spectrum that overlaps with the low-frequency flank of the boson peak. The nature of both contributions remains a subject of active discussions. Applying pressure helps to separate the temperature and volume effects on the fast dynamics. Although the boson peak under pressure was investigated recently by several groups, less attention was devoted to the fast relaxation. In this work we present the study of the fast relaxation measured in some molecular and polymeric glass formers under pressure by light (Raman and Brillouin) scattering. Different experimental conditions were applied: isothermal, isobaric, isokinetic, and isochoric. The results are analyzed within the frames of various theoretical models. In particular, the pressure dependence of the spectral shape and amplitude of the fast relaxation spectrum and the relative change of the spectrum in comparison with the boson peak makes it possible to check in detail the predictions of the soft-potential model of glassy dynamics.

Crystallization of supercooled nanodroplets

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Aerosols of nanosizes in the stratosphere serve at the seeds for the nucleation and freezing of H_2O. Some aerosols are glassy or highly viscous droplets and in generally aerosols contain hydrophilic components such as sulfate- and nitrate ions. The stability of supercooled liquid mixture is controlled by the exothermic strengthof the mixture. The binary mixture of water and sulfuric or nitric acid in the aerosols is one example. The mixture of water and sulfuric acid has an extreme exothermic strength, and it is this quality which stabilizes the supercooled aerosol as well as it controls the onset of crystallization.

A droplet of $10\ nm$ contains of the order 10^4 molecules which can be simulated (Molecular Dynamics) with today´s computers and followed over what corresponds to many μs, which is sufficient to observe crystallization in supercooled mixtures. In the first set of simulations we took the Kob-Andersen (KA) model, because their bulk behavior at low temperature is well established. In the second set of simulation we simulated a united-atom model of a binary mixture of water and sulfuric acid.

The qualitative behavior of the two models for exothermic mixtures is the same. The exothermic binding between solute and solvent molecules ensures an enhanced concentration of solute molecules in the interior of the droplet and a thin solute layer at the surface. The enhanced solute concentration in the interior of the droplet has two consequences. One: it stabilizes the supercooled system futher, and second: when the crystallization appears, it takes place near the surface and with a tendency to cover the surface like an egg-shell. This crystallization mechanism explains some important phenomena observed in polar stratospheric clouds.

A Molecular Dynamics Simulation Study of Torsional Barriers Effects in Poly(vinyl methyl ether)

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We have departed from the same system that was used in a recent work where poly(vinyl methyl ether) (PVME) was used to study the self hydrogen dynamics above the glass-transition temperature in the light of the mode coupling theory (MCT). The validation of the simulations, by neutron scattering experiments, supports this model as a reliable system on which, now, we may separately study the role of the different underlying elements contributing to atomic motions. The aim of this work was to study the effect of the torsional barriers, both, by switching them off and also by enhancing them. In the first case, (when torsions are “smoothed out”) the results were again analyzed in the light of the MCT, and a lowering of the lambda-exponent parameter was observed in agreement to what has been observed in a previous work where torsional barriers were included in a simple bead-spring model of a polymer system and the reverse effect, i. e., the increase of lambda was observed. Their bottom-up approach is inverted in our case. However, both approaches point in the same direction by hinting the close relationship that may exist between intramolecular barriers and high lambda values in polymers. We have also observed that this “switching off” of the torsional barriers can be considered for relaxing systems in order to obtain better equilibrated initial starting points to run equilibrium dynamics after torsions are restored again. This procedure is not to be compared to metadynamics or hyperdynamics, but, is shown to provide a fine maneuver to obtain better relaxed systems. The influence of torsional barriers on the gaussian character of the dynamics is eventually discussed too and we are able to assign the non-gaussian peak which usually shows up in atomistic simulations of polymers around 0.1 ps to torsional movements.

Effect of Blending on the Chain Dynamics of the "Low-Tg" component in non-entangled polymer blends

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The effect of blending on the dynamics of polymers is a relevant topic from both a technological and a theoretical point of view. The separated segmental dynamics of each component in the blend and its phenomenology have been extensively studied in the last decade. In comparison, there are fewer works dealing with the effect of blending on the individual chain dynamics of different components in a blend. Here, we have characterized the effect of blending on the dynamics of Polyisoprene (PI) - the "fast" component- in Poly-tert-butylstyrene (PtBS) blends with very large dynamic asymmetry, and at molecular weights well below the entanglement limit, focusing on the normal mode (NM) process. The overall dielectric response of PI becomes slower as the high-Tg component PtBS increases. More interestingly, there is a gradual broadening of both low and high frequency tails of the NM-relaxation. The magnitude of the broadening depends on: i) the concentration; ii) the temperature; iii) the dynamic disparity, i.e. the difference between the component´s pure Tg. Therefore, we observe a clear failure of the Rouse model in describing PI´s chain dynamics in PI/PtBS blends despite the fact that all the molecular weights involved in the system are well below the entanglement limit. This excludes more habitual interpretations based on topological size effects and point to other factors like dynamic heterogeneity in blends and its effects on the monomeric friction coefficient and memory effects. Finally, contrary to the behaviour observed in the pure homopolymer, the comparison of the characteristic times for the alpha- and NM-relaxations shows that segmental dynamics of PI component exhibits a weaker T-dependence than its terminal dynamics. This effect is more pronounced the higher the PtBS content, and as a result, the separation between the maxima of both relaxations ranges from 3 decades in pure PI and PI>50% blends, to 5-6 decades for 20%PI blends.

29 SEPT. | 15:00 | Poster Session

Intercalated molecules of variable sizes into graphite oxide at the sub-nanometric scale: confinement effects on the dynamics and crystallization.

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The use of layered materials is being actively pursued for numerous applications in electronic, magnetic, optical and structural materials. In particular, graphite oxide (GO), which is an oxygen rich derivative of graphite, has been intensively studied in last years. GO is a highly hydrophilic material and is able to intercalate diverse type of molecules in the interlayer, which varies from 5.5 to 6 Å, depending on the synthetic procedure. In this work, several molecules were intercalated into layered GO starting from very small sizes [i.e. water and organic solvents (alcohols, aromatics, chlorine compounds)] to polymers [1-3]. The study was divided into two parts, one is the effect of the intercalant in the GO structure and other is the effect of the sub-nanometer confinement on the dynamics of polymers. A general observation was the significant expansion and contraction of GO interspacing as a function of the amount of intercalated molecules, and the distortion of the stacking layers after deintercalation. From this study, valuable information about solvent-GO interactions was provided, resulting the water to be the best solvent that can be used as vehicle to intercalate polymers. Thus, water-soluble polymers were intercalated through polymer diffusion into GO interlayers in an aqueous medium. The effect of confinement on the dynamics of different water-soluble polymers was studied by means of broadband dielectric spectroscopy and differential scanning calorimetry. In particular, confined poly(ethylene glycol) showed a clear slowing down of the dynamics as compared to the bulk polymer. Finally, it was observed that the confinement of polymer chains in the GO interlayer prevented the crystallization.

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Atomistic and molecular probing of amorhous polymers in relation to neutron scattering and dielectric relaxation dynamics: Poly(vinylmethyl ether)

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We report on the annihilation behavior of the ortho-positronium (o-Ps) probe and the rotation dynamics of the smallest spin probe 2,2,6,6-tetramethyl piperidinyloxy (TEMPO) in structurally simple amorphous polymer - poly(vinylmethyl ether) (PVME) - as obtained from positron annihilation lifetime spectroscopy (PALS) or electron spin resonance (ESR), respectively. The dynamic data of these atomistic and molecular probes are related to the results from neutron scattering (NS) and broadband dielectric spectroscopy (BDS).

A number of empirical correlations between the o-Ps lifetime, tau3, and the spectral parameter of mobility and correlation time, tauc, of TEMPO with the spectral and relaxation quantities from NS and BDS have been found. Thus, phenomenological analysis of the quasi-sigmoidal tau3(T) dependence reveals four characteristic PALS temperatures: Tb1G = 0.75Tg(DSC), Tg(PALS)= 250K ~ 248K = Tg(DSC), Tb1L = 1.13Tg(DSC) and Tb2L = 1.36Tg(DSC). Similarly, phenomenological evaluation of the ESR responses gives also four characteristic ESR temperatures: TX1G = 0.74Tg(DSC), TX = 1.02Tg(DSC), TX1L = 1.12Tg(DSC) and TX2L = 1.35Tg(DSC). All these temperatures corresponds to discontinuity in the first temperature derivative of the o-Ps lifetime and the correlation time ofTEMPO. Such a discontinuity in the PALS and ESR responses of the glassy PVME at Tb1G ~ TX1G appears to be related to the fast secondary beta process from NS. Further, the slight PALS and ESR crossovers in the liquid state of PVME at Tb1L ~ TX1L are found to be related to the slow beta process from BDS. In addition, these bend crossovers are close to the crossover temperature, TXbetaKWW, in the non-exponentiality paratmer of the primary alpha process as well as to the characteristic temperatures T0(CG) and Tm,c from the extended free volume (EFV) model of Cohen and Grest or the two -order parameter (TOP) model by Tanaka. Finally, the onset of the high-temperature quasi-plateau effect in tau3(T) plot at Tb2L occurs when tau3 matches the mean structural relaxation time, taualpha. Moreover, the quasi -plateau effect is connected approximately with a crossover in the structural relaxation time from the non-Arrhenius to Arrhenius dynamic regime. On the other hand, the crossover in the TEMPO dynamics at TX2L agrees with the crossover in the slow secondary beta process. Above TX2L, the TEMPO dynamics is controlled directly by this slow secondary beta process.

In summary, all these empirical correlations indicate very close connections between the PALS and ESR responses and the internal dynamic behavior in PVME as obtained from the direct dynamic techniques and point to the importance of the understanding the latter phenomena for explanation of the former ones based on the external probe principle of the soft matter characterization.

29 SEPT. | 15:00 | Poster Session

Attractive interactions of PEO-containing block copolymer micelles in salt solutions

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A Block-copolymer comprised of a hydrophobic and poly(ethylene oxide) (PEO) block have shown to be a good model system for self-assembly studies. PEO-containing block-copolymers can form spherical micelles in water when linked to a short hydrophobic tail.[i] In the current project the attractive interactions of the micelles formed by the block-copolymer surfactant Brij700 is studied. This polymeric surfactant system is composed of about 100 ethylene oxide units with a hydrophobic tail of a C_{18} chain. For pure water, the cloud point is around 100oC, however, the addition of 0.9 M NaF or 0.7 M $MgSO_4$ lowers the cloud point sufficiently to enable the study of both the repulsive and attractive intermiceller interactions at experimentally obtainable temperatures. The block-copolymer systems have been studied as a function of temperature and concentration by turbitometry, viscometry, densiometry, and small-angle X-ray scattering (SAXS). The densiometry revealed a steep decrease in the apparent specific volume at low temperatures, further clear changes are also evident in SAXS-data. The SAXS-measurements of the block-copolymer systems have provided information on the structure of the micelles and the temperature dependence of the intermicellar interactions. In viscosity it is evident that the interparticle interaction decreases with increasing temperature corresponding to the decrease observed in the hard sphere radius and the hard sphere volume fraction found by modeling of the SAXS-data. Further from the SAXS-data a decrease in the overall size of the micelles are also observed with increasing temperature.

*[i]*Sommer, C., Pedersen, J.S., Garamus, V.M., Structure and Interactions of Block Copolymer Micelles of Brij 700 Studied by Combining Small-Angle X-ray and Neutron Scattering. (2005) L*angmuir* 21, 2137-2149

Chain dynamics in nonentangled polymer melts: A first-principle approach for the role of intramolecular barriers

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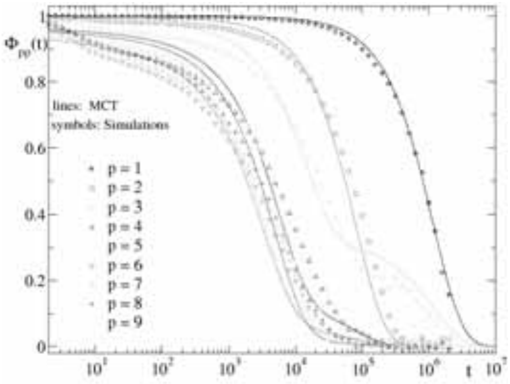
We systematically investigate the role of intramolecular barriers on the internal chain dynamics of nonentangled polymer melts. By means of molecular dynamics simulations, we study relaxation of the Rouse modes, esentially covering all the range of barrier strength between the limits of fully-flexible and stiff chains. We observe that the introduction of strong intramolecular barriers violates the Gaussianity of static and dynamic intrachain correlations assumed by the Rouse model, leading to stronger deviations from the former as chains become stiffer. In this work we rationalize deviations from Rouse behavior in semiflexible polymers within the framework of the Mode Coupling Theory (MCT). Numerical solutions of the MCT equations reproduce all the highly non-trivial features observed in the simulations for the Rouse modes by increasing the internal barriers. Such features include anomalous scaling of the relaxation times, long-time tails and plateaux, and non-monotonic dependence of the Rouse correlators on the mode wavelength (see figure below). Thus, this work provides a global microscopic picture of chain dynamics as a function of the internal barrier strength, and establishes MCT as a first-principle theory for dynamics of nonentangled chains in a large family of polymer systems.



29 SEPT. 15:00 Poster Session

Investigation of fd-virus in a temperature gradient

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Thermal diffusion or thermodiffusion is linked to ordinary, mass or molecular diffusion. Both processes have opposite effects. While thermal diffusion causes a mass separation and a redistribution of the components, mass diffusion attempts to homogenize the concentration of these components. At the steady state, both contributions counterbalance, resulting in a steady state with zero flow. The relevant magnitude of this effect is called the Soret coefficient.

Since the discovery of thermal diffusion, the effect has been observed in different fields such as geology, biology, physiology, energy and environment. In the last years, the interest in biological fields has increased such as the study of DNA thermophoresis [1] or thermotaxis, which is a mechanism guiding the mammalian sperm to the fertilization site [2].

In this study we have used the infrared thermal diffusion forced Rayleigh scattering (IR-TDFRS) technique [3] to investigate the Soret effect of a stiff filamentous virus, fd-Y21M. We have determined the mass diffusion, thermal diffusion and Soret coefficients of the fd virus in two different buffers, a) 2 mM TRIS-HCl (high Debye length), and b) 20 mM TRIS-HCl + 100 mM NaCl (short Debye length), both with a pH=8.2. Additionally, we studied the influence of temperature and fd concentration on the thermal diffusion properties.

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Tg depression and accelerated physical aging of PS in PS/Gold nanocomposites with similar dynamics: a free volume holes diffusion model interpretation

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Due to their large polymer/inorganic nanoparticles interface, polymer nanocomposites exhibit markedly modified properties when compared to bulk polymers. Nevertheless, despite the large amount of work performed, the time evolution of nanocomposites properties towards those of the equilibrium below the glass transition temperature (T_g), the so-called physical aging, still has to be clarified.[1] Indeed, physical aging results in many deleterious effects ranging from embrittlement to reduction in permeability.

Our work aims to study the effect of gold nanoparticles on the segmental dynamics, glass transition (T_g) and physical aging of polystyrene (PS). To do so, PS/Gold nanocomposites samples containing 5 and 20 wt.% of 60 nm spherical gold nanoparticles were prepared. On one hand, the T_g of PS as assessed by means of differential scanning calorimetry (DSC) was shown to decrease with increasing the amount of gold nanoparticles in the samples. On the other hand, the segmental dynamics of PS, as measured by means of broadband dielectric spectroscopy (BDS), was found to be unchanged in presence of gold nanoparticles. The equality of the segmental mobility of PS in all samples permitted to study the effect exclusively arising from the presence of gold nanoparticles on the physical aging of PS. By measuring the amount of recovered enthalpy of PS – by means of DSC – after annealing at temperatures below T_g for various aging times, the physical aging was shown to speed up with increasing the nanoparticles weight fraction, i.e. the amount of PS/Gold interface in the hybrid material. Both the significant effect of the amount of PS/Gold interface on the physical aging rate of PS and the depression of the calorimetric T_g in presence of nanoparticles, are well accounted for by the model of the diffusion of free volume holes towards polymer interfaces.[2],[3],[4]

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29 SEPT. | 15:00 | Poster Session

Computer simulations and neutron scattering experiments on the polymer blend PEO/PMMA

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We have recently reported on fully atomistic simulations on PEO validated by neutron scattering experiments and found that the system can be described using the Rouse model. In this work we will focus on MD-simulations of the dynamically asymmetric polymer blend poly(ethylene oxide) in poly(methyl metacrylate) (PEO/PMMA). Both components form a miscible binary blend despite of completely different timescales that vary by orders of magnitudes (difference in Tg of 200 K). The question is, how the presence of the slow component (PMMA) influences the local behavior of the faster polymers (PEO) and if a modification of the Rouse model introducing randomly distributed friction coefficients (random Rouse model, RRM) can describe the behavior of PEO.

The system was simulated at different temperatures (above and below Tg of PMMA) at a composition of 20 weight-% PEO in 80% PMMA. The molecular weight of both components was low (MW=2000 g/mol) in order to reach simulation times of up to 200 ns. The validity of our simulations was checked by comparing the single chain dynamic structure factor with neutron spin echo (NSE) measurements performed at the J-NSE (FRM II).

A Rouse mode analysis of the MD-simulations has shown strongly modified friction coefficients but restoring forces identical to the pure melt. The RRM can not fully describe our system as it assumes a situation where density fluctuations of the slow component are very much reduced compared to the PEO dynamics. In our case, however, the low molecular weight allows relatively fast motions of the PMMA component as we have also seen in the NSE results. In addition, a coarse grained bead spring model featuring beads with different interaction potentials was compared to the fully atomistic simulations. Despite of the much simpler approach, the generic properties of asymmetric polymer blends are represented in both systems.

Dynamics of hydration water in a Polymer system

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Water is of outmost importance in many systems, for example in biology, water seems to have a trigger role in the protein activity. This effect arise from the complex interplay between water and proteins dynamics. A first approach to understand the water dynamics in biological systems can be made by using simpler systems owning similarities with biological ones. In this direction water-polymer solutions share with biological systems some properties, the presence of a well bounded hydration layer is one of the most striking feature [1, 2]. At low hydration level, the former type is supposed to be in direct contact with the polymer chain and would exhibit a more restricted dynamics. Contrarily, at high hydration levels many of the water molecules would be bounded having a much less restricted dynamics. We have investigated the dynamics of water confined in a matrix of Polymer using two types of polymer, poly-(vinyl-pyrrolidonne) (PVP) and poly-(diméthyl-aminoéthylméthacrylate) (PDMAEMA). We follow the dynamics of both polymer and water in hydration domain where both types of water are present. Quasi elastic neutron scattering are of particular interest in this case, using isotopic substitution for water, we have been able to disentangle dynamics of each component of the system. Moreover spatial informations about the geometry of the hydrogens motions throughout the Q-dependence of the scattered intensity is also of particular interest in order to separate dynamics contributions. These experiments have been completed with other experiments, as 2H NMR, dielectric spectroscopy and DSC, allowing us to follow the dynamics of the components upon 12 orders. In both cases, the dynamics of the water show a non-Arrhenius to Arrhenius behaviour around the glass transition of the water polymer system.

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29 SEPT. | 15:00 | Poster Session

Water dynamics in a polymeric environment: a neutron scattering and dielectric spectroscopy study.

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Polymers offer a very good possibility to study water dynamics in confinement. In fact, due to their high value of the glass transition temperature, they often remain frozen in a temperature range in which the dynamics of water is relevant. Besides, polymers share similarities with biological macromolecules, so they can also be used in the wide context of understanding biological processes as model systems to investigate how water behaves in biological system and how it affects its environment. Due to the large amount of hydrogen atoms, neutron scattering (NS) is a suitable technique to study such samples. In this work a poly(vinyl methyl ether) (PVME) water solution with water percentage in weight of w_{water}=30% was studied by quasielastic NS and dielectric spectroscopy (DS) experiments. In such condition of hydration, water crystallization on cooling is prevented. Using the H/D labelling, the effects of water on the PVME structure and dynamics have been studied. The results of the NS experiments carried out on PVME/D_2O were in fact contrasted against dry PVME literature data. Then, analyzing NS and DS data obtained from the experiments performed on the PVME/H_2O sample, the investigation has been focused on the water dynamics in the polymeric matrix.

Water dynamics in cement based materials and deoxyribonucleic acid (DNA)

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The dynamics of water in confined geometries at low temperatures (110-260K) is one of the great challenges that have fascinated the scientific community due to its significant repercussion in several fields of biological, chemical and physical sciences. In particular, the dynamics of confined water is one of the hot topics in the physics of condensed matter. Recently it was reported the existence of a crossover near T_{cross} = 220K from high-T non-Arrhenius to low-T Arrhenius behavior in several systems [2a,3b,5] and interpreted as a transition from the high density to low density phase of supercooled water (fragile to strong transition - FST). The existence of this crossover is a current hot topic of debate.

In this work we present a different approach to the problem by studying two different systems: hydration water at the surface of deoxyribonucleic acid (DNA) and water in calcium silicate hydrate (C-S-H), the most important hydration product of cement based materials. In spite of the fact that these two systems are substantially different, similarities can be found in the behavior of water dynamics when studied by broadband dielectric spectroscopy (10^{-2} to 10^{8}Hz) in the low temperature range (110-280K). We will show in this work that the origin of the apparent FST can be understood in the frame of a merging between two different relaxations at T_{cross}. This experimental fact indicates that no sign of a fragile-to-strong transition happens in these two systems.

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Stable vs normal glass: to a better understanding of aging in glasses.

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When a glass ages below the glass transition temperature, it becomes denser and more stable both thermodynamically and kinetically. One of the main goals in understanding aging is to prepare glasses that have aged a very long time. The usual way is to wait for months, but this approach reaches quickly a limit because of the high relaxation times. Recently the group of Madison university succeeded in preparing a glass forming liquid in a very stable glass phase by vapor deposition [1]. Tri-naphtyl-benzene is a typical glass forming liquid with T_g= 348 K. The gas is deposed at very low rate (0.2 nm/s) on a substrate at 0.85 T_g. At this temperature, the mobility of the free molecules at the surface remains important and so the system can relax to a very stable state before new molecules recover them. The obtained glass, called stable glass, is as stable as if it has aged for some centuries [2]. We will show that the vibrational density of state and the resulting heat capacities provide new insights to characterize the stable glass as compared to normal glass and crystal. We have then performed inelastic neutron scattering experiments to understand the thermodynamic and dynamic properties of stable glass and to compare it in an ordinary glass. This gives us the elements to understand the difference between the two: we observe differences in the vibrationnal density of states (VDOS) of the 2 glasses, in the heat capacity in the heat capacity hardly seen by adiabatic calorimetry.

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Possible Natural Tuning of Protein and Water Dynamics in the Terahertz Window

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The collective dynamics of atoms, or groups of atoms, in proteins in the terahertz frequency window is supposed to be fundamental for driving functionally relevant conformational transitions on a global scale. These density fluctuations are significantly delocalised, so that they may have a role as well for cooperativity mediation in allosteric proteins. However, due to the difficulty of singling out their coherent signal from the usually large background of single-particle localised motions, the features of collective modes in proteins are still far to be completely understood. Here we report the results of a neutron spectroscopy study on the maltose binding protein where, thanks to the availability of fully deuterated samples, measured at different hydration degrees, we could obtain the first experimental determination of the dynamical contributions separately arising from the protein, the protein-water interface and the hydration water. We found that the protein is able to sustain two distinct modes in the THz range, with the same frequencies of pure water. One of these modes has a dispersive character and propagates through the whole protein-water system. It can be speculated that proteins are *naturally organised* to be dynamically coupled with water in the region of fast density fluctuations.

Nanocomposites based on Nanostructured diblock copolymers and Nanoparticles

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Block copolymers have many applications based principally on their ability to form spontaneously regular nanometre-scale patterns by self-assembly processes. These self-assembled patterns have been suggested for a proper nanoparticle dispersion and location. With these ideas in mind we have investigated systems based on nanostructured diblock copolymers of poly(styrene)–poly(dimethylsiloxane) (PS–PDMS). The morphology of these diblock copolymers has been characterized by Transmission Electron Microscopy (TEM) and Small Angle X-Ray Scattering (SAXS).

We have synthesized gold (1) and iron oxide nanoparticles (2) which have been properly functionalized (3) in order to promote the preferential location in the PDMS phase. The morphology of the resulting materials has been characterized by means of TEM and SAXS. We are also interested in studying the influence of the nanoparticles on the dynamics of the PDMS phase which has been previously studied in the absence of the nanoparticles.

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Effect of osmolytes and Hofmeister salts on protein adsorption

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In a biological cell, proteins perform their functions in a highly complex environment comprising crowding and confinement effects as well as interactions with interfaces, cosolvents, and other biomolecules. Cosolvents can stabilize or destabilize the native folded structure of proteins in solution. Here, we present recent studies on how ionic and non-ionic cosolvents affect the interfacial affinity and structure of proteins at hydrophilic and hydrophobic surfaces [1,2]. We studied the adsorption of bovine ribonuclease A (RNase A) at the silica-water, the polystyrene-water, and the air-water interface as model systems that were analyzed applying optical reflectometry as well as neutron and X-ray scattering techniques. The degree of protein adsorption and the density profile of the adsorbed protein films were determined in the absence and the presence of cosolvents. It has been found that both the protein stabilizing glycerol and the destabilizing urea cause a distinct reduction in the interfacial affinity of RNase A, which may represent a rather unexpected result. At the hydrophobic polystyrene surface, it has been found that both the kosmotropic salts, $(NH_4)_2SO_4$ and Na_2SO_4, and the chaotropic salts, NaSCN and $Ca(SCN)_2$, significantly reduce the amount of adsorbed protein, while maximum adsorption is observed in the presence of NaCl.

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Lignin/carbon nanotubes composites with low percolation threshold

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Percolation in carbon nanotube composites is of high interest because of the potential to obtain electrically conductive systems, with low mass of particles. That is, the conductivity dramatically increases in a system with low concentration of carbon nanotubes, following the classic scaling law of percolation theory.

The present study deals with the synthesis of polyurethane-lignin co-polymer to be used for all-solid-state potentiometric chemical sensors. Lignin is biopolymer formed by the phenylpropane units and contains a variety of functional groups lending it ion exchange properties and making it an attractive active substance for the chemical sensing. Co-polymerization of lignin with isocyanate should allow fixing of the former inside the polymer and thus ensuring high stability of the sensing material.

We report the d.c. electrical conductivity and the dielectric properties at frequencies between 40 Hz and 100 MHz, in the temperature range -100 to 100 ºC, of the lignin/carbon nanotubes composites with different concentrations of the dispersed conducting particles.

The percolation model theory was used to describe d.c. and low frequency behaviour, where the electrical conductivity and the dielectric constant are expressed by scaling laws, near the threshold conduction. In this case, the material presents a very low critical concentration of 0.18 %.

The dielectric analysis was made using the modulus formalism, and the dielectric relaxation behaviour modelled by the Cole-Cole expression. The calculated relaxation parameters show that, with the increasing concentration of carbon nanotubes, the system becomes more heterogeneous, which is confirmed by the broader distribution of the relaxation times.

Poster Session | 15:00 | 29 SEPT.

Investigation of the hydration water and internal dynamics of biocompatible and not biocompatible polymer

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Biocompatibility of polymeric materials, i.e. the ability to resist protein and cell absorption, is of crucial concern when designing new materials to be used for biomedical applications. The mechanism behind biocompatibility is not yet understood, and it is thought that, among other factors, the hydration water plays a major role in it. In this work we investigate how the dynamics of hydrated polymers changes according to their biocompatibility, hydration and temperature. We started this comparative study using two different newly synthesized poly-(ethylene glycol) (PEG) based polymers. Poly(2-methoxyethylacrylate) (PMEA), which shows an excellent biocompatibility against platelets, white blood cells and proteins [2]. Poly[2-(2-ethoxyethoxy)ethyl methacrylate] (PEEA), a thermosensitive polymer, whose ability to resist protein and cell adsorption is expected to vary in the room temperature region.

Elastic and quasielastic neutron scattering experiments were performed to reveal the internal dynamics of polymers hydrated in H2O and D2O in an extended time and length scales. The samples had an equilibrium water content not far from saturation and were investigated at four distinct temperatures: 200K, 263K, 277K, 310K. Preliminary results suggest that the internal dynamics is affected by the degree of biocompatibility of the polymer. Hydration does not seem to significantly influence the polymer dynamics of the biocompatible PMEA as a function of temperature, while a clear effect is observed in the thermosensitive PEEA polymer. In order to shed light on this aspect, an investigation on a non bio-compatible PEG polymer (chosen as negative control), the di-block copolymer poly(MEA-2-hydroxyethylmethacrylate) is in progress . The results will be discussed in the context of biocompatibility of polymer materials.

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29 SEPT. | 15:00 | Poster Session

Dynamics of DPPC Vesicles in the Presence of Bioprotectants

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Biological systems must often be stored for extended periods of time. This is done by lyophilisation in the presence of lyoprotectants, such as sugars, which results in stable products at ambient conditions.[1] In an effort to understand the mechanism of preservation and stabilization, the interactions between sugars and liposome vesicles, which serve as a simple membrane model, have been studied extensively. Amongst the common sugars, trehalose has superior preservative effects [1] and accumulates to high concentrations in many anhydrobiotic organisms.

Despite many experimental and numerical studies three mechanisms are proposed: vitrification [2], preferential exclusion [3] and water replacement [4]. To gain more insight into the stabilization mechanism we have recently investigated the effect of trehalose on the bending elasticity of fully hydrated unilamellar vesicles of 1,2-dipalmitoyl-phosphatidylcholine (DPPC) in D_2O at temperatures below and above the lipid melting transition (Tm) using neutron spin-echo. The data was analyzed using the Zilman-Granek theory. At all temperatures measured, trehalose stiffens the bilayer suggesting strong interactions between trehalose and the lipid. Trehalose appears to broaden the melting transition but does not change the Tm. This agrees with observations using differential scanning calorimetry.

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Dynamical properties of the blend of polyvinyl acetate with its trimer

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During the last years, the dynamics of polymer blends have attracted a lot of attention for the peculiar behaviour exhibited, for example the existence of dynamical heterogeneity [1]. An enhancement of these unusual properties is observed if the asymmetry in the system is increased by either choosing components with very different glass-transition temperatures or asymmetric compositions, leading even to the emergence of confinement effects for the minority component. Exotic behaviour in the dynamical properties of several real blends, and also a bead-spring simulation of a polymer blend with high dynamic asymmetry [2] have been reported. In this work we have investigated the structural and dynamical properties of a blend of polyvinyl acetate (PVAc) with its trimer at different temperatures above as well as below the experimentally determined glass transition of the blend (Tg(blend)=260 K). This system shows a marked dynamic asymmetry (Tg(Trimer) = 209 K, Tg(PVAc)=314 K) and also composition asymmetry (30%Trimer), therefore we expect to show confined-like behaviour of the trimer in the neighbourhood of the effective glass-transition temperature of the polymer component. In our study we have combined neutron scattering and fully atomistic molecular dynamics simulations. The neutron study was carried out on a sample with deuterated polymer in order to isolate the information relative to the trimer component. The simulation results have been validated by comparison with the experimental data. Thereafter, the contributions of both components to the dynamical properties have been analyzed and interpreted with the help of the simulations.

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Current status of BioSAXS beamline at PETRA-3

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Small angle X-ray and neutron scattering techniques are complementary methods in studies of soft bio matter i.e., polymers and surfactants in solutions. Now GKSS Research Centre operates few SANS1 machines and REF-SANS machine at FRM II reactor. In nearest future GKSS will expand the research field to SAXS. Together with EMBL Hamburg, GKSS is building BioSAXS beamline at upgrated PETRA-3 ring (3rd generation synchrotron source). New SAXS instrument will be ready in 2010 and opens new opportunities in the structural studies of solutions.

A Molecular Dynamics simulations study on the Structure and the Dynamics of polyisobutylene.

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By means of fully atomistic molecular dynamics simulation we have investigated the structure and dynamics of the glass-forming polymer polyisobutylene (PIB) at temperatures well above the glass-transition. A system of 20 chains of PIB of 70 monomers each, being in total 16800 atoms in a cubic cell, was constructed and subjected to periodic boundary conditions. The simulations were carried out at 500K, 470K, 390K, and 365K extending until 20 ns. We first calculated the incoherent intermediate scattering function of all the hydrogens and the dynamic structure factor, i.e., the magnitudes accessed by previous neutron scattering results on protonated and deuterated samples. The direct comparison of our results with the existing experimental data allowed us to validate the simulated cell. Taking advantage of the simulations, we calculated thereafter magnitudes that are difficult or cannot be experimentally accessible, e.g. the mean squared displacement and the second-order non-Gaussian parameter for different C and H atoms (main chain and methyl groups). Questions like the relationship between collective and self-motions, and how does the dynamic structure factor behave in the intermediate length scales region were also addressed.

29 SEPT. | 15:00 | Poster Session

Study of the phase separation of non-miscible polymer blends by using Electrostatic Force Microscopy

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Polymer thin films consisting of single component and multi-components are of great interest because their properties are very different from bulk, and directly related to many important surface phenomena. In particular, phase separation in thin films of non-miscible polymer blends has recently created great interest. One of the most useful approaches typically used for studying the polymer distribution in thin films is atomic force microscopy (AFM). This technique is very versatile and allows measuring the size and distribution of the different phases in heterogeneous polymer blends. However, AFM measurements are typically limited to topographic or phase imaging which give partial information about the distribution of the polymer chains in the blend. To overcome this constrain we have studied the phase separation in non-miscible polymer blends using a recently developed experimental approach that allows imaging the local dielectric permittivity of thin films by means of electrostatic force microscopy (EFM). This experimental method is based on the detection of both, the topography and the electric force gradient at different values of the tip-sample distance. In this way we are able to image both the topography and the dielectric permittivity of polymer thin films obtaining complemental and useful information. In this work we analyse by means of EFM the phase separation of thin films of polystyrene (PS) and poly (vinyl acetate) (PVAc) blends with different thicknesses and thermal treatments. We will show that the dielectric response not only is fully decoupled from the topography, but also gives additional information about each polymer phase as well as the interphase.

Water and Polymer Dynamics in Wet Polyamides

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Absorption of water and in general polar solvents on polyamides has the effect of strongly reducing their mechanical properties and changing the application properties during the lifetime of manufactured parts. The understanding of the adsorption mechanisms and the influence of water on dynamics are therefore of fundamental importance in order to develop barrier properties to solvents.

By combining inelastic neutron scattering and broadband dielectric spectroscopy measurements we explore the effect of water adsorption on the dynamics of polyamide samples with largely different degree of crystallinity. We observe a plasticizing effect of water on the segmental relaxation of the polymer accessed by dielectric spectroscopy. On the other hand the fast processes at low temperatures show a suppression of local dynamics with addition of water, as evidenced by neutron scattering experiments.

Confined water dynamics are observed below Tg of the mixture, while above the dynamics are substantially diffusive, but characterized by a distribution of relaxation times related to the different environment explored by water. In addition, by comparing data for materials with largely different degree of crystallinity, we can distinguish a pronounced effect of the crystalline phase on water dynamics both below and above Tg: Relaxation times are found to increase of approximately an order of magnitude in the presence of a large degree of crystallinity.

29 SEPT. | 15:00 | Poster Session

Local and medium range structures in supercooled colloidal liquids and their link with dynamics: confocal microscopy study.

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A glassy state of matter results if crystallization is avoided upon cooling or increasing density. The dramatic slowing down of the dynamic is often thought as decoupled from any structural change. However, the possibility of a correlation between medium range crystalline ordering and the dynamic heterogeneities which characterizes the glass transition was brought into light by recent simulations and 2D driven granular matter experiments. Using hard-sphere like polydisperse colloids tracked in real space by confocal microscopy, we are able to extract both structural and dynamic information at the particle level. We indeed detect transient medium range crystalline order but also more local icosahedral order frustrating further crystallization. Our data seem to suggest a mutual exclusion between theses two types of ordered clusters and the fast dynamics regions.

Structure and dynamics of polymer coated gold nanoparticles

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Polymer-capped gold nanoparticles (AuNP) have many peculiar aspects like quantum size effects and single electron transitions. Their properties are highly dependent on their size and shape and upon spatial relationship of one particle to another. Coating nanoparticles with polymers tethered to their surface by means of specific ligands stabilizes them, and allows functionalization for specific applications in nanotechnologies, biology and biomedical studies, and can promote the bottom-up approach to the fabrication of nanostructures.

We studied the structure and the dynamics of a key class of polymer-capped AuNP, those coated with poly ethyleneglycol (PEG AuNP). A novel synthesis was developed by ligand exchange procedure, which ensure the production of NP with little excess of (expensive) functionalizing ligand and high stability. When dissolved in water, PEG AuNP are typical example of mesoscopis solute in microscopic solvent and the thermodynamic conditions of the solution depend on the extension and local properties of the solute-solvent interfaces.

The structure PEG AuNP were studied by combining small angle neutron scattering (SANS) and other techniques as a function of temperature, and of the length of the interfacial polymer chains. PEG Au NP functionalized with short (PEG400) and long (PEG2000) polymer reflected substantial differences in the structure of the polymer at the interface. A significant effect due to the solvent isotopic substitution was also envisaged. The dynamics of PEG AuNP in the nanosecond timescale was also studied by neutron spin echo (NSE) spectroscopy. NSE experiments gave evidence of two dynamical processes, one related to the translational diffusion of the nanoparticles, and a faster due to internal motion of the polymer chains. For comparison, NSE experiments were performed on PEG2000 polymer in solutions. Analogies and differences between free and anchored polymer will be discussed.

29 SEPT. | 15:00 | Poster Session

Water cluster breaking ions

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The effect of solutes on the water structure, has been a topic of intense research since the early days of physical chemistry. We looked at the hydrogen bonded clusters made up by water molecules in several solutions over a range of concentrations, by combining neutron diffraction data with computer modeling. Here we show that the relative viscosity of a solution is related to the size of the largest water cluster. The value and sign of the viscosity B-coefficient are determined by the difference between the oxygen-oxygen distance in pure water and the ion-oxygen distance in solution. Therefore, no solute can be considered as water structure maker, as all solutes break down the hydrogen bonded water cluster. Moreover, the size of this cluster breaking effect is simply due to the solute ability to draw in or draw out water molecules.

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The distribution of the Dynamically Accessible Volume simulated with Bond Fluctuation Model

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Bond Fluctuation Model[1] is one of the most frequently used models for polymeric materials. That model reproduces distribution of relaxation times characteristic of segmental mobility of an amorphous polymer[2]. Since relaxation times become longer as the temperature decreases, calculation of relaxation times requires more and more simulation time as temperature approaches the glass transition. This makes difficult to reach conclusions on the temperature dependence of the width of the relaxation times distribution.

In this work we show how additional information can be obtained from Dynamically Accessible Volume[3]. Once a static image of the structure of the simulated system has been obtained, the accessibility of the empty sites of the lattice can inform about segmental diffusion[4]. Because of the relationship between diffusion coefficient and relaxation times, it is possible to calculate the distribution of Dynamically Accessible Volume and compare it with the distribution of relaxation times. We have found that the distribution of the Dynamically Accessible Volume in an amorphous system becomes narrower as temperature decreases.

The study of Dynamically Accessible Volume distribution confirms the existence of domains with different mobility, which will help to understand processes such as glass transition and structural relaxation. This method allows calculating the dynamics of the system from a single static image, and accurately representing the evolution of the system when it is out of thermodynamic equilibrium, simply using a representation of the system at successive instants of time.

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29 SEPT. | 15:00 | Poster Session

Acoustic modes in glasses and the breakdown of the Debye approximation

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The Debye approximation for the acoustic modes in crystals is based on the assumption that the medium is an elastic continuum. This holds true for wavelengths much larger than the typical interatomic distance and gradually breaks down on approaching the microscopic scale. In glasses the structural disorder undermines this approximation in a subtle way, still not completely clarified.

Using molecular dynamics simulations of a model monoatomic glass of very large size, we show that the breakdown of the Debye approximation appears in glasses quite abruptly. It shows up as a significant reduction of the sound velocity with respect to the macroscopic value, on the mesoscopic length-scale of the order of ten interatomic spacings. We also show that this features allows us to rationalize the ubiquitous excess over the Debye level found in the specific heat of glasses at low temperatures.

G. Monaco and S. Mossa, Proc. Natl. Acad. Sci. USA *106*, 16907 (2009)

Influence of topology on effective potentials: coarse-graining ring polymers

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We employ computer simulations and integral equation theory techniques to perform coarse-graining of self-avoiding ring polymers with different knotedness and to derive effective interaction potentials [1] between the centers of mass (CM) of these macromolecular entities. Different microscopic models for the monomer-monomer interactions and bonding are employed, bringing about an insensitivity of the effective interactions on the microscopic details and a convergence to a universal form for sufficiently long molecules.

The pair effective interactions are shown to be accurate up to within the semidilute regime with additional, many-body forces becoming increasingly important as the polymer concentration grows. The dramatic effects of topological constraints in the form of interaction potentials are going to bring forward and critically discussed [2].

We further perform topology-preserving Monte-Carlo simulations of many ring polymers using the blob representation. Effective interaction potentials between CM of linear chains are used between blobs. These allow us to simulate more and bigger molecules, reaching higher concentrations and saving computational time. We compare results from the blob picture and monomer resolution, so we can establish the rage of validity for blob technique, and also study the effect of topology for big ring polymers at moderate densities.

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29 SEPT. | 15:00 | Poster Session

Role of Methyl Groups in Dynamics and Function of Biomolecules

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Recent studies reveal significant differences between the dynamics of proteins, DNA, and RNA connected to methyl group rotation. Methyl group rotation is known to function as an intrinsic plasticizer in synthetic polymers. We suggest that methyl groups are acting as critical intrinsic plasticizers in biomolecules as well. An immediate implication of this observation is the recognition that early life based on RNA for both catalysis and gene storage would have lacked methyl groups and subsequently, lacked these dynamic processes. This is a new perspective with which to consider the progression of biomolecule evolution. The evolution of RNA (no methyls) to DNA (a few methyls) and from nucleic acid based ribozymes to protein based enzymes (many methyls) introduced methyl groups to the biomolecular repertoire. The inclusion of methyl groups into the structure of biomolecules opened up the availability of lower activation energy dynamics and the associated increase in molecular flexibility. From this perspective one of the major functions of methyl groups is facilitation of the protein dynamics as an intrinsic plasticizer. Therefore, we would expect different methyl group content and spatial distribution in proteins which require different relative flexibility for their function. Indeed, extracellular matrix proteins that provide structural support (such as collagen and fibrinectin) have significantly lower methyl content (per molecular weight) than most enzymes, which require flexibility and active dynamics to catalyze reactions. The presented analysis of several proteins also reveals that the location of the most mobile methyl groups (those on methionine, isoleucine, and leucine side chains) appears frequently around active sites. This approach developed by nature can be employed in Materials Science for the design of novel functional and ‘smart’ soft materials.

Poster Session | 15:00 | 29 SEPT.

Spin contrast variation technique for neutron scattering measurement of softmatters

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Contrast variation technique is a powerful tool for the structural analysis of multi-component systems. For small-angle neutron scattering (SANS) experiments, the scattering length density can be controlled by deuterium substitution or proton spin polarization. For polarizing proton spins, we generally use a technique of dynamic nuclear polarization (DNP), which results from transferring a large spin polarization from electrons to nuclei, thereby aligning the nuclear spins to the extent that electron spins are aligned. Recently, we investigated the effect of dynamic nuclear polarization (DNP) of proton spins on small angle neutron scattering (SANS) from a block copolymer (bcp) composed of polystyrene (PS) and polyisoprene (PI) block chains (PS-b-PI) as an ideal system having well designed microphase-separated materials. As a source of an electron spin for DNP, 2,2,6,6-tetramethylpiperidine 1-oxyl (TEMPO) was doped into the PI microphase. The SANS profile showed the 1st, 2nd and 3rd order peaks due to the periodic lamellar structure of the bcp. By DNP, the change of the peak heights was successfully observed. Furthermore, the proton spin polarization dependence of the peak heights agreed precisely with the theoretical prediction. Since TEMPO radical spontaneously permeates softmatters which generally has a fluid phase, we propose that spin contrast variation study with TEMPO vapor doping is widely applicable for softmatters.

29 SEPT. | 15:00 | Poster Session

Novel polymeric micelle-like structures assembled by metal ion addition designed for radiopharmaceutical purposes

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We synthesized and studied properties of novel biodegradable micelle-like structures made from graft copolymers assembled by the addition of metal ions and carried out biological tests on them. The polymer structures are composed of a graft polymer consisting of backbone chelating polymeric chain poly(*N*-methyl methacryloylhydroxamic acid) with hydrophilic poly(ethylene oxide) grafts. The backbone polymer chain is able to bind essential metal ions (Fe^3+ or Cu^{2+}), which serve as bioreversible crosslinkers. These metals may be transchelated directly or after reduction to lower oxidation states (Fe^2+ and Cu^1+) inside cells, but at the same time the chelate bond is sufficiently stable during the transport in blood. The metals are though biologically trapped inside the cell and the polymeric chain can be eliminated from the body. The polymer also enables to bind a suitable metal radiolabel – such as ^{64}Cu – for imaging in radiodiagnostics of malignancies.

Targeting of the polymeric structures into tumor tissue is based on the enhanced permeation and retention (EPR) effect. The EPR effect causes passive accumulation of macromolecular drug delivery systems in solid tumors, thanks to their leaking vasculature and missing lymphatic drainage. Our polymeric structures have sufficient molecular weight to exhibit EPR effect and are designed to decompose (after fulfilling their task) into particles with molecular weights under renal threshold so they can be eliminated by kidneys.

Financial support of the Grant Agency of the Czech Republic (grants # P207/10/P054 and 202/09/2078) is gratefully aknowledged.

Interfacial water dynamics in simple oligopeptides

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Water is undoubtedly quite interesting for a number of reasons, and in particular in the supercooled metastable phase. While experimental studies on bulk supercooled water are extremely difficult, hydration water on the surface of proteins can provide a valuable alternative, because the binding of water molecules to the protein substrate avoids crystallization. Actually, several factors limits a detailed experimental investigation of water dynamics in a protein-water system, such as the intrinsic low solubility of proteins in pure water, and the chemically and topologically disordered surface of the large protein macromolecules. For these reasons, the use of model systems such as water solutions of small oligopeptides, build up by few aminoacids with either an amphiphilic or hydrophilic character, represent an excellent way to almost eliminate topological disorder and to investigate the role of chemical heterogeneity in well defined local environment.

In this work, as a model for protein-water interaction, we use water solutions of glutathione (GSH), a simple amphiphilic tripeptide, that in the intracellular medium acts as an antioxidant, helping to protect cells from reactive oxygen species such as free radicals and peroxides. Broadband dielectric spectroscopy (BDS) and differential scanning calorimetry (DSC) measurements were performed on glutathione water solutions, revealing a quite complex dynamical behaviour for this system. Differently form hydrophilic glass forming water containing systems, where two dynamical phenomenon are normally observed (a slower, non-Arrhenius, one, attributed to the collective movements of the system and a faster, Arrhenius-like, one, due to water molecules), here at least four relaxation processes are present at all hydration levels. Two of these relaxations are assigned to water-related molecular motions, while the other two phenomena, appearing well above the calorimetric glass transition temperature, seem to be connected to the polypeptidic nature of the solute, being previously observed in a hemoglobin water sample.

LAOS: a new signature for the mechanics of filled elastomers

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The Payne effect is the classical denomination of small strain-softening observed in elastomers containing solid particles – as used in car tires. In the literature, only the amplitude of the modulus is measured as a function of the strain amplitude.

Here we present recent LAOS (Large Amplitude Oscillatory Shear) results on filled elastomers consisting of a dispersion of silica particles into a polymeric matrix. A sinusoidal strain was applied to the samples and the corresponding stress was measured and analyzed. With increasing strain, we observed a decrease in the storage modulus - the Payne effect, but also other types of non-linearity. In order to analyze the signals, we first used the method proposed by Cho et al. to decompose the stress into an elastic part and a viscous one.

During a single cycle of LAOS, we could observe ***simultaneously*** **strain hardening** reminiscent from a finite extensibility phenomenon and **strain softening** - the usual Payne effect.

Both seem to be correlated in our model samples and to come from the local strain amplification between the particles.

Chain Dynamics of Poly(ethylene-alt-propylene) Melts. Bridging the Gap between Fully Atomistic and Coarse-grained Simulations

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In order to better understand the dynamic features in the region between atomic motions and chain dynamics, i.e., between segmental and Rouse regime, we present coarse-grained (CG) simulations of Poly(ethylene-*alt*-propylene) (PEP) melts. These simulations consist of a bottom-up approach to construct an appropriate CG model of PEP (R. Pérez-Aparicio et al., J. Chem. Phys. 132, 024904 (2010)), developed by Prof. Briels' group. The CG parameters, potential of mean force and bare friction, were determined from fully atomistic MD simulations carried out on a PEP cell containing 12 chains of 80 monomers each (each chain was replaced by a set of 8 *blobs*, each of them containing 10 monomers), subjected to periodic boundary conditions and previously validated by neutron scattering measurements. Uncrossability constrains were also introduced in the CG model to prevent unphysical bond crossing. The simulations were carried out at 492 K focusing on chain dynamics, ranging in chain length from about M_e (the entanglement $M_{w)}$ to $M_w=6M_e$. The results obtained were analyzed in the framework of the Rouse model. We observe deviations from Rouse behavior for all chain-lengths investigated, even when the chain-stiffness is incorporated in the Rouse model. These deviations become more important as the chain-length increases. The general scenario emerging from the results obtained is that the deviations from Rouse-like behavior are directly driven by the uncrossability algorithm, which produces correlations among the forces acting upon a chain bead and as consequence, non exponentiallity of the Rouse correlators and mode- and time-dependent friction. It seems that in the M_w range explored these effects give not raise to reptation behavior yet but to a crossover regime between Rouse and reptation. On the other hand, the results obtained are in qualitative agreement with those expected from the so-called generalized Rouse models, based on memory function formalisms.

29 SEPT. | 15:00 | Poster Session

Scaling law cross-over during the the collapse of polydisperse chains to unimolecular nanoparticles: Effect on SEC polysispersity

POMPOSO José A.[1], PEREZ-BAENA Irma[1], ALEGRIA Angel[2, 3], COLMENERO Juan[1, 2, 3]

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SEC - size exclusion chromatography - is a technique very valuable to distinguish macromolecules according to their hydrodynamic radius (R_H) and hence to quantify the R_H size distribution of a given sample. When combined with well-known Mark-Huggins theory, access to the sample molecular weight (M) distribution is achieved. As expected, a significant reduction in R_H is found by SEC upon intramolecular collapse (by cross-linking) of individual polymer chains to unimolecular particles. Surprisingly, a concomitant reduction in polydispersity is often observed by SEC even when the actual molecular weight distribution remains unaltered. We demonstrated here that this unusual behavior can be rationalized by taking into account the different size scaling laws for random coils ($R_H \sim N^{1/2}$, where N denotes the number of chain segments) *versus* compact spheres ($R_H \sim N^{1/3}$). A general expression providing the maximum potential molecular weight reduction upon collapse (M_{app}) has been derived, that for polystyrene (PS) nanoparticles reduces to $M_{app}(PS) » 15 \times M^{2/3}$. The general expression has been employed to quantify the degree of chain collapse from several experimental systems reported in the literature. Finally, theoretical decrease in SEC polydispersity upon coil-to-nanoparticle collapse has been calculated for several illustrative molecular weight distributions.

Dielectric and mechanical properties of polymers at macro and nanoscale

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This presentation will summarize the research of my Phd Thesis. The idea was first to understand the physical theories that describe the dynamics of linear polymers at the macroscopic scale. Rouse and the reptational tube theory describe the large scale dynamics of unentangled and entangled polymers respectively. Using Broadband Dielectric Spectroscopy (BDS) and rheology we have studied the different transitions between these two regimes. Avoiding the segmental relaxation contribution and introducing a distribution of molecular weight we have been able to perform a comparison of the Rouse model with dielectric and rheological data (Macromolecules **42(**21): 8492-8499). Effects of entanglement on dielectric spectra will be discussed (Rheologica Acta. 49(5):507-512). Then we have developed EFM-based methods in order to study the local dynamics. Using the numerical simulation of the Equivalent Charge Method, the value of the static dielectric permittivity has been quantified from the measurement of the force gradient created by a V_{DC} potential between a tip and a grounded dielectric (Journal of Applied Physics **106(**2):024315). This method allows a quantitative mapping of dielectric properties with a 40 nm spatial resolution and is therefore suitable for the study of nano-defined domains (Physical Review E 8**1(**1): 010801). The electrical phase shifts in the 2ω components of the force or force gradient created by V_{AC} voltage, $\Delta\Phi_{2\omega}$, are related with dielectric losses. Measuring the frequency dependence of $\Delta\Phi_{2\omega}$ Crieder e*t al* (Applied Physics Letters 9**1(**1):013102) have shown that the dynamics at the near free surface of polymer films is faster than the one in bulk. We have used this method in order to visualize the activation of the segmental relaxation with temperature and frequency (Applied Physics Letters **96(**21): 213110). All this measurements can be achieved using a standard Atomic Force Microscope.

Phase Diagrams of Tetrahedral Patchy Colloids: role of the interaction range and patch width

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I will present recent results regarding the thermodynamic behavior of tetrahedral patchy colloidal particles, exploring the role of the range of interaction and the angular width of the patch on the phase diagram.

The phase diagrams shows a variety of crystal phases and an interesting competition between gas-liquid separation and crystallization. By comparing the different thermodynamic behavior of the fluid and the crystal phases and their dependence on the range and angular patch width, I will infer information on how to best design tetrahedral patchy colloidal particles which self-assemble into a diamond-crystal structure, a structure particularly relevant for photonic applications.

Coarse-graining polymers with the MARTINI force-field: polystyrene and polystyrene nanocomposites

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We propose a hybrid thermodynamic-structural approach to the coarse-graining of polymers. The new force-field is derived within the framework of the MARTINI [Marrink *et al.*, J. Phys. Chem. B, 2007, **111**, 7812] model, conventionally applied to the study of biomolecules. We refine the MARTINI parameterization to better reproduce the change of polymer conformation induced by the environment, the latter being a melt or a solvent. The force-field optimization is mainly based on the reproduction of experimental data.

We test our procedure on polystyrene, a standard benchmark for coarse-grained polymer force-fields. The model preserves the backbone-ring structure of the molecule, each monomer being represented by four coarse-grained beads. Structural properties in the melt are well reproduced, and their scaling with chain length agrees with available experimental data. The relatively fine degree of coarse-graining we have adopted allows for a realistic description of the inter-molecular friction. The time conversion factor of the CG model with respect to atomistic simulations is constant over a wide temperature range. The model results to be transferable in the 350-600 K range. Polystyrene melts can be simulated over length scales of tens of nanometers and time scales of tens of microseconds. Collapse and swelling of the polymer chains in a bad and a good solvent, respectively, are observed.

The model is applied to the study of the dynamics of polystyrene-C_{60} nanocomposites.

Direct measurement of dynamical correlation length reveals nontrivial behavior.

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We study the supercooled liquid state of the hard-core N3 lattice gas model (square lattice with exclusion up to 3rd nearest neighbors). The model undergoes a first order transition at activity $z_c \approx 40$, and the analysis of the Mayer cluster integral expansion predicts termination of the super cooled liquid branch at finite activity $z_t < z_c$ with termination density lower than the closest packing density[1]. We conduct a Monte Carlo study to provide evidence for glassy behavior of the density-density correlation. Both the β regime plateau and the α regime stretched exponential decay are observed. The β plateau time increases and seem to diverge at density close to ρ_{rcp} [2]

In a further study the 4 point correlation function $G_4(r,t)$ is measured and shows a growing correlation length. Our measurement shows that in this simple model the 4 susceptibility χ_4 peak time τ_4, is determined not by the maximum of the dynamical correlation length ξ_4 but by shorter range dynamic correlations. We further show that in short times contribution to χ_4 is global and is replaced later by correlated regions.

[1] Z. Rotman and E. Eisenberg Critical exponents from cluster coefficients, Phys. Rev. E 80, 031126 (2009)
[2] Z. Rotman and E. Eisenberg Ideal glass transition in a simple 2D lattice model , Phys. Rev. E 80, 060104(R) (2009)

On the behaviour of water hydrogen bonds at biomolecular sites: dependences on temperature and on network dimensionality

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Neutron scattering experiments have been used to investigate the effects of temperature and network dimensionality (from hydrated powders to highly concentrated solutions) on the hydrogen bond dynamics of hydration water molecules at specific sites in selected biomolecules. With this aim in view, the evolution of hydration water dynamics of a prototypical hydrophobic amino acid with polar backbone, N-acetyl-leucine-methylamide (NALMA), and a hydrophilic amino acid, N-acetyl-glycine-methylamide (NAGMA), has been investigated as a function of temperature.

We show that the temperature dependence of the diffusive dynamics of water molecules is the same for both hydrophilic and hydrophobic peptides. A comparison between hydrated powders and high concentrated solutions reveals a similar behaviour, particularly for the hydrophobic peptide. On the other hand we find a distinct difference in the behaviour with temperature of the hydrogen bond lifetime in solutions and hydrated powders. Whereas at room temperature the hydrogen bond lifetime is longer in solution than in the hydrated powder, the reverse situation obtains at low temperatures.

The measured and calculated low-energy vibrational densities of states of hydrated powders show significant shifts of the peak position to higher energy and a decrease of the amplitude which corresponds to an apparent lower temperature as compared with bulk water. Both effects are more pronounced for the hydrophilic peptide, which confirms that the dynamics of hydration water is similar to that of bulk water at lower temperatures and that the "plasticity" of the hydrogen bond is larger in hydrophobic environments.

29 SEPT. | 15:00 | Poster Session

Oligonucleic acids (“aptamers”) for designing stimuli-responsive membranes

SCHÄFER Thomas[1], ÖZALP Cengiz Veli[2]

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This work explores the feasibility of designing selective and tunable interfaces for sensors and membrane separations based on oligonucleic acids which are to be employed in downstream processing and monitoring. Oligonucleic acids (“aptamers”) are biomolecules that can be designed to specifically interact with in principle any kind of target molecule, similarly to what is known from antibodies. Contrary to the latter, however, the chemical stability of oligonucleic acids is far greater, and the screening for the aptamer with a desired selectivity toward a particular target can be done by an automated in vitro selection procedure. As a consequence, interfaces based on these selective compounds should allow reducing the costs of production significantly compared to antibodies, while maintaining a high selectivity.

An important asset of oligonucleic acids is the fact that upon specific binding, their spatial conformation may change drastically, allowing in principle their use for stimuli-responsive sensing or separations, with the stimulus being actually target compounds rather than conventional stimuli such as pH, light and/or temperature.

In this study particular attention is given to the potential of using oligonucleic acids to selectively interact with small molecules, which has hardly been explored until today. It is shown how aptamers may specifically interact with targets as small as ethanol amine, a low molecular weight carcinogenic compound, as well as adenosine triphosphate. However, possible pitfalls in the application of oligonucleic acids in separations will also be stressed clearly, mainly related to the fact that being complex biomolecules their changes in spatial conformation may not be independent of the feed composition.

It will be demonstrated that target-specific oligonucleic acids can nevertheless be a promising alternative to existing methods of creating selective, stimuli-responsive interfaces, particularly with respect to their versatility and their potential to be designed for virtually any target molecule.

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Ionic liquids as emerging materials in membrane separation and purification - hype or proven potential?

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Room-temperature ionic liquids are salts that commonly are liquid at ambient temperature owing to steric hindrance, resulting in a negligible vapour pressure. As a consequence, they have been intensively studied as alternative, benign solvents and catalysts for chemical reactions in the context of sustainable chemistry. Another main asset, however, is the theoretical possibility of designing virtually any type of ionic liquid for specific purposes. Owing to the fact that there are practically no limits to vary the affinity and physico-chemical properties of ionic liquids by introducing suitable functional groups and altering their chemical structure, they have more recently emerged as supposedly selective materials for membrane separations, gas sequestration and purification.

Despite the tremendous physico-chemical variety which is attributed to ionic liquids, however, it can be seen that in practice either one and the same group of ionic liquids is employed for very distinct tasks, or different ionic liquids are employed showing very little discrepancy in their selectivity – a trend which strongly contradicts their alleged potential.

This presentation therefore aims at discussing the performance of room-temperature ionic liquids in the context of the selectivity of conventional materials used in separations, such as polymers, and separation challenges such as the sequestration of carbon dioxide. Molecular simulations as an indispensable tool for the selection of specific ionic liquids are presented and compared with experimental data on selectivity and permeability, highlighting also the pitfalls one encounters when putting theoretical predictions into practice. Eventually, it will be resumed and elucidated in how far ionic liquids may be considered as strong alternatives to existing materials in separations, and which are the cases where they most probably will always be prone to fail.

A starting-grant from the European Research Council (no. 209842-MATRIX) is gratefully acknowledged.

The Effect of Asymmetric Component Mobility on Static Properties in the PEO/PMMA Blend

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A symmetric 25kDa binary polymer blend poly(ethylene oxide) PEO and poly(methylmethacrylate) (PMMA) was examined by small angle neutron scattering (SANS) in a temperature interval between 10 and 150°C. This system is of particular interest as the glass transition of both polymers occurs at very different temperatures thereby inducing a dynamic asymmetry in the elementary molecular dynamics of the two components. The Flory-Huggins parameter was determined via random phase approximation (RPA) from the degree of thermal composition fluctuations which also determined the transitions to the glass and crystallization phases at low and high PEO content, respectively. The radii of gyration of the two components were obtained from blends of proper isotope choice. The SANS experiments were supplemented by DSC and dynamic shear measurements on the same samples.

PEO/PMMA is miscible at the given temperatures and the disordered regime is separated by a so-called gelation temperature T_A into two parts with distinctively different Flory-Huggins parameters. Phase separation is expected at high temperatures roughly above 400°C. A large isotope effect of gelation as well as of glass transition temperature is found for the blend whereas T_G of PMMA is the same whether protonated or deuterated. This means that the observed shift of T_A and T_G with the choice of the PMMA isotope must be caused by the PEO component. We also observed a slight streching of the PEO chain when passing T_G. The SANS data, e.g. the susceptibility were interpretated within the theory of "Dynamical Asymmetry" as developed in refs. [1,2] and compared with the dynamic shear modulus from the same melts.

[1] A. Onuki, Phase Transition Dynamics, Cambridge University Press, Cambridge 2002.
[2] M. Doi and A. Onuki, J. Phys. II (France) **2**, 1631 (1992).

nanoDielectric Spectroscopy (nDS) of polymeric systems by using Electric Force Microscopy

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Broadband dielectric spectroscopy (BDS) has shown to be a powerful technique to study the molecular dynamics of polymers and glass forming systems over a huge frequency range (10^{-5}–10^{12}Hz) at different temperatures, pressures and under different environments. Although their well known exceptional features, the standard BDS techniques have a fundamental limitation: *they provide no spatial resolution*. To overcome this constrain we have been developing during the last years different approaches[2-5] that allow mapping the local dielectric permittivity of thin films by means of electrostatic force microscopy (EFM) with typical spatial resolution of about 20nm. The proposed experimental methods are based on the detection of both, the topography and the electric force gradient at a given value of the tip-sample distance. In this way we are able to image both the topography and the dielectric permittivity of polymer thin films. Besides the success of these methods they were limited to measure the static dielectric permittivity.

In this work, we present an extension of those methods to measure the local frequency response of thin films. Thus, by means of a standard AFM setup, we are able to measure both, the local dielectric loss spectra over more than four decades in frequency (2-3.210^{4}Hz) and the dielectric contrast image at a given frequency and temperature. We have tested our method on several systems; we have measured the segmental relaxation on both pure polymers and nanophase-separated polymer mixtures, the secondary relaxation on poly(methyl methacrylate) and the polymer dynamics in nanocomposites. This method seems to be an appropriate tool for approaching fundamental problems of soft matter and will open the door for studying the complex dielectric response in polymers, nano-structured materials, biological systems and soft matter in general.

29 SEPT. | 15:00 | Poster Session

Dynamic Heterogeneity in Diblock Copolymer

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We present extensive computer simulations on the dynamics of a simple bead-spring model for diblock copolymers in the lamellar phase. This constitutes a well-known example of systems exhibiting confinement effects, due to the strong interfacial barriers separating consecutive lamellar layers. We investigate the case in which the two blocks are characterized by very different intrinsic mobilities, i.e, the corresponding homopolymers exhibit very different glass transition temperatures. We present a detailed characterization of the dynamic features of this system. These include the role of the distance to the interface on monomer translations and bond reorientations, as well as the influence of the interface on the relaxation of the chain normal modes (Rouse modes). Results are presented for several values of the lamellar spacing and the interfacial energy.

Dynamics @ Interfaces: New, highly sensitive methods for characterization of soft matter

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How do the dimensions of a film in the nano- to micrometer range influence its dynamic properties? How does the presence, structure, chemistry, etc. of a solid interface influence the motion of particles in solution, polymer chains, membranes, etc. The answer to these questions is vital for our understanding of soft matter in this partly controversial discussed field. Evanescent wave in total internal reflection techniques combined with dynamic light scattering have been developed in the past. These lack species selectivity, in situ monitoring of changes of the interface itself, and have a generally weak signal. To overcome these problems we have developed methods utilizing surface plasmon polaritons and metal enhanced leaky waveguide modes as incident fields in light scattering experiments. These new, highly efficient methods have been succesfully applied to some of the questions risen above and will be presented in the presentation.

29 SEPT. | 15:00 | Poster Session

Conductive Properties of Inorganic/Organic Nanostructured Polymeric Materials Using Electrostatic and Tunneling Force Microscopy

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The main aim of this work was the generation of novel smart materials, in this case thermo and electro-responsive inorganic/organic meso/nanostructured hybrids based on different low molecular weight liquid crystals (LC) and conductive rutile TiO_2 nanoparticles as well as amphiphilic poly(styrene-b-ethylene oxide) block copolymers (PS-*b*-PEO) as matrix. LC as partially miscible with polystyrene (PS) was well-dispersed using PS-*b*-PEO block copolymers. Simultaneously, LC was used as surfactant for conductive rutile TiO_2 nanoparticles. Relation between morphology generated and thermo and electro-responsive properties of designed systems was investigated used atomic force microscopy (AFM). AFM images were obtained operating in tapping mode (TM, Nanoscope IIIa scanning probe microscope (Multimode ™, Digital Instruments) and Nanoscope IV (Dimension 3100, Digital Instruments)). The ability of alignment of liquid crystal phase and electrical properties of TiO_2 nanoparticles were studied by **electrostatic force microscopy (EFM)** (Nanoscope IV (Dimension 3100, Digital Instruments)) and **tunneling atomic force microscopy (TUNA)** (Nanoscope IV (Dimension 3100, Digital Instruments). Additionally, electrical response of the nanocomposites was measured using a semiconductor characterization system (K**eithley model 4200-SCS**).

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Molecular dynamics of poly-alkyl-thiophenes: experimental study by neutron scattering, rheology and calorimetry

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Poly-alkyl-thiophenes are conjugated polymers which have been widely used as active layers in organic electronic devices such as field-effect transistors, organic light emitting diodes and organic solar cells [1]. In particular, blends of P3HT and functionalized fullerenes in tandem devices have been the most successful realization of the bulk-heterojunction concept in which two interpenetrated networks of materials perform as electron donors or acceptors [2]. The morphology of the blends is strongly correlated with the performance of the devices, but a deep understanding of the molecular dynamics of these polymers at different temperatures is still lacking. We will present a detailed study carried on solutions and bulk samples of P3OT and P3HT, the experimental techniques that we have used include quasielastic neutron scattering measurements in pulsed (OSIRIS instrument at ISIS-RAL, UK) and continuous neutron sources (IN10 instrument at ILL, France) as well as calorimetric and rheological studies of the same samples. Our findings include the description of a low temperature glass transition, the characterization of the side chain and backbone dynamics, and the experimental determination of the crystallinity of the samples. We will also present the potential of other neutron scattering techniques such as small angle neutron scattering (SANS) and neutron reflectivity in the study of the structure and dynamics of polymeric multilayered organic electronic devices [3, 4].

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29 SEPT. | 15:00 | Poster Session

Synchrotron SAXS Study of Micelle Formation

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In the present study we report unique investigations of the kinetics of formation of micelles from a *non-equilibrium* solution of singly dissolved surfactants. Using synchrotron radiation SAXS at the ID02 beamline at ESRF, time-resolved measurements of the process is investigated.

The non-ionic surfactant dodecyl-maltoside is singly dissolved in pure DMF at the investigated concentrations. However, in a 1:1 DMF/water mixture micelles are observed at concentrations above 0.7 mg/mL. The starting non-equilibrium system for the synchrotron measurements was obtained by rapid mixing a solution of dodecyl-maltoside in DMF with water using a stopped-flow cell. The three investigated concentrations were only slightly above the critical micelle concentration (cmc), leading to relatively slow kinetics of the micelle formation which allowed it to be followed *in sit*u.

For the two lowest concentrations no micelle scattering was detected in the first several measurements (see figure 1a) and the experiment thus captures the entire process of micelle formation.
The data sets were modelled as combinations of scattering from singly dissolved surfactants and ellipsoidal micelles. The aggregation number of the initial micelles is close to 20 and then increases rapidly to the final value of ca. 50. This indicates that only aggregates above a critical size are energetically favourable and will grow to give the final equilibrium micelles. The fraction of the surfactants aggregated into micelles can be crudely fitted by a sigmoidal growth (see figure 1b). The characteristic time of the growth decreases with total surfactant concentration whereas the width of the growth region does not seem to be much influenced. Comparison to more sophisticated kinetic models is in progress.

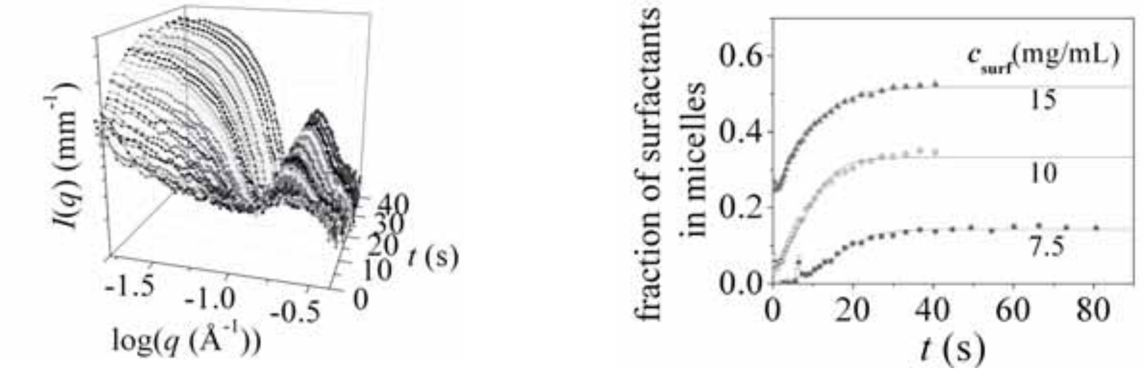

Figure 1. **a**: Scattering curves for c_{surf} = 10 mg/mL. **b**: Fraction of the total surfactant concentration in micelles as function of time. The times for the growths are 1.(2), 7.(4) and 15.(7) seconds respectively.

Complex polymer assemblies

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Hierarchical assemblies of polymers form via a wide variety of equilibrium and out-of-equilibrium routes giving rise to nanostructured objects with complex structural and dynamical properties. For example, electrostatically driven co-assembly of two oppositely charged double hydrophilic block copolymers in aqueous solutions results in core-shell micelles with a mixed core, consisting of polyelectrolyte blocks, and a mixed corona, consisting of neutral solvent-swollen blocks. The miscibility of the shell-forming blocks, and thereby the extent of chain mixing / segregation in the micellar corona, can be tuned by, for example, segment chemistry and solvent quality, yielding so-called onion-type, Janus-type, and raspberry-like micelles depending on the relative abundance and compatibility of the polymer blocks. Aggregates of protein molecules are another intriguing example of complex polymer assemblies. In vivo, they may be anything from vital - think of for example actin and tubulin polymerization - to rather detrimental as is the case in protein condensation diseases, such as sickle cell anaemia, cataract, and Alzheimer´s disease. In food and other industries, control over protein stability, aggregation, and gelation is necessary in the development of products with a desired appearance, texture, taste, and function. One way of influencing a protein’s stability is via addition of an organic solvent to an aqueous protein solution. This method has allowed us to study protein unfolding, self-assembly, and gelation processes in some detail.

29 SEPT. | 15:00 | Poster Session

Model PI-PDMS Block Copolymers - Synthesis, Characterisation and Physical Properties

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Model polyisoprene-polydimethylsiloxane (PI-PDMS) block copolymers have recently been used to study the PI-dynamics under soft confinement by broad band dielectric (BBS) [1] and neutron spin echo spectroscopy [2]. The soft confinement was achieved by self-assembly of the PI-PDMS block copolymers which was either spherical [1] or cylindrical [1,2] depending on the composition of the PI-PDMS block copolymer. The general outcome of these studies is an acceleration of the PI-dynamics within the domains compared to the dynamics in a pure PI homo polymer which is essentially explained by fluctuations of the interface between PI and PDMS.

In this work we present a systematic study of the dynamics in different geometrical confinements, i.e. spherical, cylindrical and lamellar. For this purpose a series of block copolymers has been prepared by sequential living anionic polymerization and characterised by a combination of NMR, multi angle laser light scattering, membrane osmometry and size exclusion chromatography in toluene and THF. The synthetic pathway including the non-trivial characterisation as well as the synthesis of corresponding deuterated species will be presented. The morphological characterisation was done by small angle x-ray scattering. Results will be shown on the poster. Furthermore, preliminary results obtained by BBS will be presented and discussed.

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Amorphous ices – the glassy states of water

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An understanding of the numerous anomalies of water is closely linked to an understanding of the phase diagram of the metastable non-crystalline states of ice[1]. Since the discovery of high- (HDA) and low-density amorphous ice (LDA) [2] the question arose if this phenomenon of polyamorphism may directly lead to the occurrence of more than one supercooled liquid.

For LDA the calorimetric glass→liquid transition shows the existence of a low-density liquid (LDL) at ambient pressure, whereas for HDA such an experimental proof has been missing so far. We here present calorimetric measurements on HDA, showing for the first time that HDA transforms into a liquid upon heating even at ambient pressure.

Differential scanning calorimetry (DSC) is an established experimental method to investigate vitrification and devitrification transitions between glasses and liquids. The glass→liquid transition upon heating is evidenced by an endothermic step, which indicates that the liquid has a higher heat capacity than the glass due to increased molecular mobility. In the case of water, such a glass-softening endotherm has already been observed for hyperquenched glassy water (HGW) as well as for LDA [3]. Previous calorimetric experiments on HDA were performed on unrelaxed HDA (uHDA), without any sign for an endothermic glass-softening. Using a relaxed form of HDA [4,5], the glass→liquid transition HDA→HDL is astonishingly detectable at ambient pressure. Our findings strengthen the two-liquid theories of explaining water anomalies.

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29 SEPT. | 15:00 | Poster Session

Exchange kinetics in n-alkane-poly(ethylene oxide) block copolymer micelles

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We report on an experimental study of the equilibrium kinetics in model block copolymers C18-PEO5k and C24-PEO5k having a monodisperse hydrophobic block. By recent time resolved small angle neutron scattering (TR-SANS) measurements by Lund et al. have shown, that the relaxation curves follow a logarithmic time dependence [1] in contradiction to the single exponential time decay predicted by theory. Recently, Choi et al. could explain this logarithmic time law for the chain exchange between the micelles by taking into account the polydispersity of the core forming block [2]. The aim of this work is to verify this results with a monodisperse model system.

For the TR-SANS experiments two pairs of deuterated and hydrogenated block copolymers with similar molecular characteristics, h-C18-h-PEO5k, d-C18-d-PEO5k, h-C24-h-PEO5k and h-C24-d-PEO5k, were prepared. The micellar properties of these block copolymers were determined in different DMF / water mixtures (DMF mole fraction 0 % – 20 %) by SANS. The dimensions of the micelles R_c and R_m as well as aggregation number P are extracted from the data by a core-shell model fitting. Results of this analysis will be presented on the poster. Preliminary kinetic results on the C24-PEO5k system reveal very fast chain exchange. In the presence of DMF solvent mixture the kinetics could not be followed. In pure water however chain exchange slows down such that kinetics can be resolved by TR-SANS. First evaluations of these results will be discussed on the poster.

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PASSION FOR PHOTONS

ABSTRACTS

Plasmonics: nanoscale manipulation of light

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Metallic nanoparticles, used since antiquity to impart intense and vibrant color into materials, have more recently become a central tool in the nanoscale manipulation of light. This interest has led to a virtual explosion of new types of metal-based nanoparticles and nanostructures of various shapes and compositions, and has given rise to new strategies to harvest, control, and manipulate light based on these structures and their properties. Light coupled to metallic nanoparticles induces collective oscillations in the conduction electrons of the structure, known as surface plasmons. As one begins to assemble metallic nanoparticles into useful building blocks, the striking parallel between the plasmons of these structures and wave functions of simple quantum systems is universally observed. Simple nanoscale assemblies of metal nanoparticles take the role of plasmonic "artificial molecules", establishing a guiding principle that allows us to predict and even design their color and properties. Clusters of metallic nanoparticles behave like coupled oscillators or antenna arrays, introducing effects characteristic of systems as diverse as radio frequency transmitters and coupled pendulums into light-manipulating structures. These paradigms give rise to new optical properties not realized in traditional materials and devices, which allow us to manipulate light in entirely new ways. These effects can be harnessed for applications that can benefit society, in applications ranging from biomedicine to energy to environmental remediation. The application of plasmonic nanoparticles to cancer cell ablation and tumor remission is a highly promising new light-based therapy already in clinical trials. New light-induced therapies allow us to address disease at the genome-altering level, and provide a research tool to examine how cells respond to induced changes in their genetic machinery in real time. Applications in areas such as alternative energy and environmental remediation are also being avidly pursued, making this bottom-up optical science one of the key areas for technological advancement in the 21st century.

29 SEPT. | 09:00 | Keynote Lecture

Photonics with nanohybrids

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Photonic cavities are commonly used to enhance and control the coupling of light to quantum emitters such as atoms and quantum dots. Dynamical control of the coupling to light is highly desirable for applications using quantum emitters as active optical sources for nanolasers and LEDs, single and entangled photon sources for quantum information processing, as sensors and detectors, and as photon collectors in photovoltaics. Nanohybrid structures that couple quantum dots to the plasmons in metal nanoparticles or that integrate quantum dots with nanomechanical structures provide new paradigms for achieving dynamical control of the coupling between light and quantum emitters. I discuss our theoretical efforts to understand the optics of these novel nanohybrids. I show how coupling quantum dots to metal nanoparticles can lead to Fano resonances in the optical response, exciton-induced-transparency, and enhanced, suppressed or bistable quantum dot response. I will also show how the strong near-field response of the metal nanoparticles and structures can be engineered to manipulate this coupling and to control nanoscale transfer of photons between emitters. Mechanical strain provides the coupling to modify quantum dots embedded in nanomechanical structures. I will discuss the understanding that we have developed of how such interaction can be used to manipulate quantum dot excitons, tune their energies, fine structure splittings, polarization and phase, and control the quantum optics of quantum dots.

From Electronics to Metatronics to Graphene Metamaterials

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In my group, in recent years we have introduced and been developing the concept of “metatronics”, i.e. metamaterial-inspired optical nanocircuitry, in which the optical displacement current (dD/dt), in-stead of conventional drift of the charged particles, play the important role as the quantity of interest for the information processing at the nanoscale. In such a paradigm, the nanostructures with specific values of permittivity may act as the lumped optical circuit elements such as optical nanocapacitors, nanoinductors and nanoresistors. The collections of such properly designed nanostructures provides a new photonic circuit platform in which optical signals can be manipulated, thus allowing optical in-formation processing at the nanoscale [N. Engheta, Science, 317, p. 1698 (2007)]. Through a variety of analytical techniques and computer simulations, and through a set of experiments at the IR wave-lengths, we have demonstrated that such optical nanocircuitry may lead to a novel platform for tailor-ing and manipulating optical signals at the nanoscale. We have also shown that in metatronics one can utilize the concept of permittivity-near-zero metamaterials as optical “nanocircuit boards” for “dD/dt wires” at optical frequencies, effectively resembling the analogous role of metallic wires in electronics as conduits for drift of charged particles [A. Alu and N. Engheta, Phys. Rev. Letts., 103, 143902 (2009)]. As “electrons” have played the crucial role in “electronics”, “photons” in “photonics”, and “spins” in “spintronics”, the optical fields and optical displacement currents in metamaterial nanos-tructures can play an equally important role in the field of “metatronics”, leading to the possibility of nanoscale data processing. We have now extended this concept to other platforms such as graphene, which is a single atomically thin layer of carbon atoms, with exciting features in electronic transport. Since the graphene has an unusual conductivity function, it does possess exciting optical and elec-tronic properties. We are exploring the concept of metamaterials in graphene as a ‘flatland’ (“zero-thickness”) platform for optical metamaterials, leading to the concept of graphene metamaterials and graphene transformation optics (A. Vakil and N. Engheta, manuscript in preparation). I will discuss some of our recent results on these topics.

01 SEPT.	09:00	Theory

Insights on surface plasmons from quantum mechanics

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In this talk I will review some of the efforts to describe the collective excitation of valence electrons in nanoscale systems within time dependent density functional theory (TDDFT). The effects of quantization, anisotropic and symmetry-dependent screening, coupling and damping of surface plasmon resonances are illustrated in model nanosystems such as linear atomic chains, thin films and nanoparticle dimers. Comparison with classical modeling and experiments are made whenever possible, which sets the limits and validity of local dielectric functions in describing the plasmonic response at nanometer scales.

Photons and electrons team up

GARCÍA DE ABAJO Javier [1]

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Optical excitations in nanostructures are finding important applications in biosensing and information technologies. These advances rely on the ability to mold the flow of visible and near-infrared light over distances much smaller than the free-space wavelength. Exquisite control over photon energy (better than one part in 107) has been possible for a long time, and so has spatial control (better than one tenth of the wavelength) using surface modes such as plasmons. However, there is a shortage of tools capable of analyzing and/or generating optical excitations with the simultaneous combination of nanometer spatial resolution and sub-meV energy resolution. Here, we will describe recent achievements in this direction, relying on the coupling between photons and electrons that is mediated by the presence of nanostructures. Examples of plasmon mapping and plasmon generation will be presented using cathodoluminescence, electron energ-loss, and electron energy-gain spectroscopies.

30 SEPT. | 10:20 | Electrons and Photons

Controlling the flow of surface plasmons

GARCÍA-VIDAL Francisco J. [1]

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In this talk we will review two different routes for controlling the flow of surface plasmons (SPs) at metal surfaces. First, we will show how the concept of spoof SPs [1] (introduction of a periodic modulation on a metal surface at a length scale much smaller than the wavelength) can be used to tailor the propagation characteristics of SPs in the optical and telecom regimes [2], to create new types of SPs as, for example, domino plasmons [3] or to transfer the capabilities of SPs to lower frequencies as microwaves or terahertz [4]. Second, we will demonstrate how the idea of Transformation Optics can be applied to the propagation of SPs [5], yielding to recipes for the refractive index map that can lead to several SP-functionalities as SP-shifters, SP-bends, SP-concentrators and lenses and to cloaking devices for SPs.

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Scattering-type Scanning Near-Field Optical Microscopy

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The development of novel nanoscale materials, composites and devices requires ultrahigh-resolution microscopy tools for characterization and mapping of local material properties and nanoscale confined light fields. In this talk, I will demonstrate a near-field optical microscopy technique providing a spatial resolution of about 10-20 nm independent of the wavelength. It is based on elastic light scattering from the probing tip of an atomic force microscope (scattering-type near-field optical microscopy, s-SNOM [1]). Besides an introduction of the technique, I will demonstrate some s-SNOM applications including infrared and terahertz mapping of chemical composition, free-carrier concentration in semiconductor nanodevices [2], strain fields and nanocracks in ceramics [3], as well as the visualization of the near-field oscillations of optical and mid-infrared plasmonic nanoantennas [4].

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Photons and Electrons – Tightening Their Embrace

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The marriage of photons and electrons, consummated in quantum electrodynamics, requires continuing efforts to deliver the best offspring with practical applications. Plasmonics and Near Field Optical Microscopy, in so far as they utilize surfaces and tips with suitable dielectric properties originating from the behaviour of their electrons, are outstanding results of such efforts. Electron microscopists, depending for their high spatial resolution on the relatively strong interactions of the electron and the revolutionary progress in electron optics, are likewise investigating various possibilities of harnessing photons for improved spectroscopy. Still more dramatic opportunities are opening up in using pulsed photon beams for ultrafast electron microscopy both in single shot imaging and pump-probe stroboscopic imaging. Amongst the many potential applications for these developments it seems most relevant in a photonics workshop to discuss some of those in the photosynthesis systems (both natural and artificial) and in photovoltaics.

Nanoplasmonic sensing: refractive index, SERS and optical forces

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Nanoplasmonic sensors can be based on a variety of transduction principles, in particular changes in plasmon resonance condition caused by a variation in interfacial refractive index and Raman scattering enhanced by plasmonic fields. I will illustrate refractive index sensing using recent experimental results on a variety of nanostructures [1] and address the fundamentally important question to what extent sensors based on localized plasmons in metal nanostructures can provide advantages over standard flat-surface SPR sensors [2]. I will also discuss plasmonic sensing based on SERS, in particular in the context of optical forces and laser tweezing [3]. Finally, I will show that it is possible to sense colloidal interactions between single Au nanoparticles based on confinement in a polarized optical potential well.

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Correlative electron and optical spectroscopies of metallic nanostructures and applications in nanometrology

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Metallic nanostructures provide a unique means for electromagnetic energy localization on the nanoscale. This presentation will discuss our recent efforts into correlative electron and optical spectroscopies of a variety of nanoassemblies supporting both bright and dark localized surface plasmon modes. Examples using colloidal assembly as well as top-down nanolithography for nanostructure assembly will be presented, examined using electron energy loss and optical dark-field spectroscopy. A deeper understanding of the observed mode spectra is obtained via full-field electrodynamic as well as electron energy loss modelling.

The nanoscale field localization can then be employed as a unique tool for nanometrology. As an example, we will present a study of phase transitions observed using nanoparticles as local probes.

Fano resonances in plasmonic nanostructures

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Plasmonic nanostructures such as narrow plasmonic cavities, strongly interacting nanoparticle aggregates, and hybrid plasmonic/excitonic systems offer highly tunable platforms for the study of radiative interference and coherence effects such as subradiance, superradiance, and electromagnetically induced transparency (EIT). In structures with reduced symmetry, narrow Fano resonances can appear in their extinction spectra resulting from the interference between superradiant and subradiant modes. Apart from their fundamental importance, such phenomena are also of practical interest in metamaterial and chemical and sensing applications because of the extraordinarily narrow linewidths and strong sensitivities to the dielectric properties of the environment. In this talk, I will present a general framework for the description of radiative interference effects in plasmonic systems and illustrate the concepts with examples from recent applications to symmetry broken nanoshells, Fanoshells [1], small nanoparticle clusters of D_{6h} symmetry (Heptamers) [2], planar ring-disk systems (Fanocavities) [3], plasmonic heterodimers,[4] and quantum plasmonics and plexcitonics".[5]

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Nonlinear Plasmonics with Optical Antennas

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Sub-nanometer variations in the geometry of optical antenna structures can have a very strong influence on their optical response. This effect is particularly strong in the nonlinear regime. We form an optical antenna in the form of two gold nanoparticles rigidly joined together. When irradiated with high intensity laser radiation, the nanoparticle junction gives rise to nonlinear frequency mixing, such as harmonic generation, two-photon luminescence, and four-wave mixing (4WM).

We will demonstrate that the nonlinear response at a gold nanoparticle junction defines a localized, tunable, and narrow-band photon source, which can be employed for high-resolution imaging and spectroscopy. The wavelength of the 4WM signal can be tuned over a wide spectral range and the process can be turned on and off by controlling the temporal overlap between the excitation pulses. The ability of switching on and off localized photon sources can find applications in nanophotonics and the emerging field of active plasmonics.

Transformation Optics at Optical Frequencies

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Transformation optics tells us how a distortion of space, and the objects it contains, maps into changes of the effective electric and magnetic responses of the distorted materials. This can be exploited to generate new devices from familiar ones. For example it is well known that a slab of negatively refracting material has lens like properties and can focus light. However the images are always of exactly the same size as the objects. This restriction can be lifted by applying transformation optics to create a negatively refracting magnifying lens that also has the property of sub wavelength. In the exact formulation both electrical and magnetic properties are equally affected by the transformation, but in the near field approximation at optical frequencies we can neglect the magnetic component. This leads to some novel devices that will be described in this talk.

29 SEPT. | 12:20 | Concepts in Optics

Plasmon nano-optics: Designing novel nanotools for Biosciences and Medicine

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Metallic nanostructures supporting localized surface plasmon (LSP) resonances have the potential to act as efficient point-like sources of both light and heat, opening plenty of new science and applications in areas ranging from integrated optics to biomedicine. In this talk, we describe our recent advances in the engineering of both the optical and thermal properties of plasmonic nanosystems and discuss their respective applications to biosciences.

The first part of the talk focuses on the subwavelength control of the optical confinement in ensembles of electromagnetically coupled nanostructures [1]. We then illustrate the applicability of the optimized structures to ultra sensitive sensing of small molecules [2] and to nano-optical trapping and optical inspection of biological systems [3,4].

In the second part of the talk, we discuss both theoretically and experimentally the general physical rules for optimizing heat generation in plasmonic nanostructures [5]. We then discuss the applications of functionalized point-like heat sources to the stimulation of intra cellular processes and cancer cell destruction.

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Resonant Optical Forces on Metallic and Dielectric Nanoparticles

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Light forces on small (Rayleigh) particles are usually described as the sum of two terms: the dipolar or gradient force and the scattering or radiation pressure force. The scattering force is traditionally considered proportional to the Poynting vector, which gives the direction and magnitude of the momentum flow. However, as we will show, when the light field has a non-uniform spatial distribution of spin angular momentum, an additional scattering force arises as a reaction of the particle against the rotation of the spin. This non-conservative force term is proportional to the curl of the spin angular momentum of the light field [1]. We will illustrate the relevance of the spin force in the particular simple case of a 2D field geometry arising in the intersection region of two standing waves [2]. The unusual properties of the optical forces acting on particles with both electric and magnetic response will also be analyzed [3].

We will also discuss the peculiar particle dynamics in the non-conservative force field of an optical vortex lattice [4]. Radiation pressure in the vortex field (arising in the intersection region of two crossed optical standing waves [2]) plays an active role spinning the particles out of the whirls sites leading to a giant acceleration of free diffusion. Interestingly, we show that a simple combination of null-average conservative and non-conservative steady forces can rectify the flow of damped particles. We propose a "deterministic ratchet" stemming from purely stationary forces [4] that represents a novel concept in dynamics with considerable potential for fundamental and practical implications.

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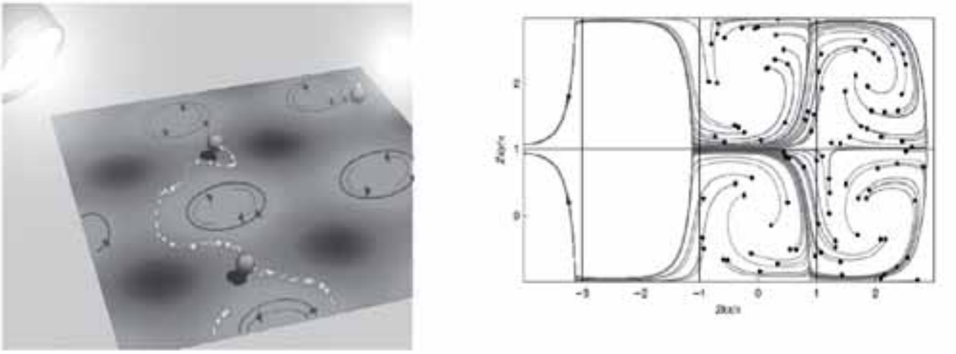

Left: Sketch of a nanoparticle enhanced diffusion path in an optical vortex lattice [4].
Right: Particle trajectories in a "deterministic"optical ratchet. Initial positions are random within the chosen unit cell. All paths converge to two limit periodic trajectories which flow to the left [5].

Trends in Nanoplasmonics: Ultrasmall, Ultrafast, Ultrastrong

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Nanoplasmonics deals with collective electron dynamics on the surface of metal nanostructures, which arises as a result of excitations called surface plasmons. The surface plasmons localize and concentrate optical energy in nanoscopic regions creating highly enhanced local optical fields. They undergo ultrafast dynamics with timescales as short as a few hundred attoseconds. From the latest developments and original work in nanoplasmonics, we will consider SPASER (quantum nanoscale optical generator and ultrafast amplifier), ultrafast coherent control on the nanoscale, generation of EUV radiation by plasmonic enhancement, adiabatic nano-concentration of optical energy, and SPIDER (surface-plasmon-induced drag-effect rectification) that leads to generation of nanoscale THz fields by femtosecond polaritonic pulses in metal nanowires.

Plasmonic-tuned microstructured optical fibers for localized surface plasmon resonance (LSPR) sensing

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Plasmonic nanoparticles with spectral properties from the UV- to the near-infrared range offer a large potential for the development of innovative optical devices. On the other hand, microstructured optical fibers (MOFs) represent a promising platform technology for fully integrated next-generation plasmonic devices. Therefore, the combination of MOFs with plasmonic nanoparticles would open the way of novel applications, especially in sensoric applications. We will demonstrate a cost-effective technique for the preparation of well-defined plasmonic layers of selected particles inside the MOFs´ channels. The presented technique leads to a longitudinal homogenous particle density as long as several meters. By using particles with defined plasmonic properties such as the resonance wavelength fibers with particle-adequate spectral characteristics can be prepared. The application of such fibers for refractive index sensing was demonstrated and yielded a sensitivity of about 78 nm/RIU. The novel, plasmonically tuned optical fibers with free selectable, application-tailored optical properties present extensive possibilities for applications of localized surface plasmon resonance (LSPR) sensing.

A nano-optical Yagi-Uda antenna driven by a quantum dot

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Nanoscale quantum emitters interact weakly and omnidirectionally with freely propagating light. As a result, efficient optical excitation and detection of such emitters involves large solid angles. On the other hand, antennas effectively mediate the interaction of propagating waves with localized energy. Here, we present unidirectional nanoscale photon sources based on the coupling of a single quantum emitter to a nanofabricated Yagi-Uda antenna. Recent experimental and theoretical results are compared.

A quantum dot is placed in the near field of the antenna through a combination of two steps of e-beam lithography and chemical functionalization. This accurately positioned emitter drives the resonant feed element of the Yagi-Uda antenna. The resulting quantum-dot luminescence becomes highly directed to a single forward lobe and strongly polarized.
We demonstrate how the antenna, that is only a single wavelength long, must be appropriately tuned by fabricating and characterizing the performance of antennas of different size parameters. Finally, we assess the dependence of the directivity on emission wavelength (bandwidth).

Unidirectional optical antennas provide a new route to effectively communicate light to, from, and between nano-emitters, with applications in single-photon sources for quantum optical technologies, planar biochemical sensors, and light-harvesting and emission devices.

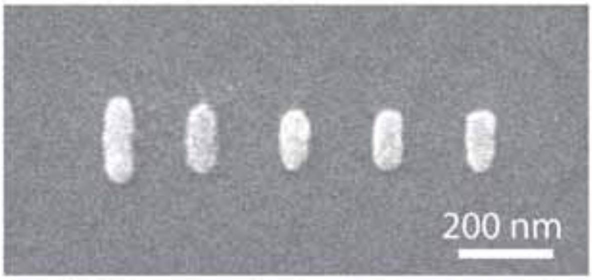

Fig. 1. Scanning electron microscopy image of a 5-element Yagi-Uda nanoantenna.

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Plasmon polariton nano-antenna for Single Molecule Detection

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The interaction occurred in recent years between physics, biology and nanotechnology has opened the possibility to investigate single molecule. This would allow the opportunity to study the chemical and structural characteristics of a protein in its environment. Membrane proteins are usually hard to crystallize and it is very difficult to obtain structural and chemical information on how these proteins change their conformation in response to ligands, agonists and drugs. In order to understand fundamental biological processes, we should be able to know: the 3-dimensional structure of membrane proteins, such has receptors and ion channels; how they change their conformation following the binding of transmitters, hormones, drugs and signaling molecules. In this work we present a new generation of devices able to: manipulate the unknow molecule; measure its mechanical properties; obtain its chemical signature and correlate all these information at a molecular level. This is made possible by combining information obtained by Raman and AFM measurements within the same chip. The device consists in a silver cone acting as a plasmonic nanoantenna, placed at the centre of a photonic crystal (PC) cavity (Fig.1, device is fabricated on AFM cantilever). The PC cavity produces an efficient coupling between the external optical source and the nanoantenna, in fact, direct coupling of the far field to the nanoantenna in the absence of a PC is inefficient, as we observed both theoretically and experimentally. The nanoantenna placed at the cavity centre supports SPP modes and acts as a nano-scale waveguide, able to propagate and focus the SPP towards the tip where strong enhancement of the e.m. field intensity occurs[1]. The geometry of nanoantenna, plays a key role in the degree of resolution obtained by measuring RAMAN. Indeed, it was demostred[2,3] that, if the shape is perfectly conical an incurs an adiabatic behavior. This causes the SPP field being effective for scattering emission only at the tip where an enhancement factor of about 10^3 for the electrical field is theoretically reachable. Such stringent conditions force the choice toward *top-down* fabrication techniques that guarantee a strict dimensional and geometrical control. The whole device was fabricated[4] using an FEI Nova Nanolab 600 dual beam system. The photonic crystal consisted of a triangular lattice of air holes (lattice constant a= 250 nm, d= 160 nm) patterned on a 100-nm-thick Si_3N_4 membrane. Three missing holes in the centre generated a photonic crystal cavity, termed L3, tuned at λ=532 nm. To fabricate the cavity on the AFM cantilever with a thickness of 100 nm, we thinned locally a commercially available Si_3N_4 cantilever (600 nm standard thickness) around the area of the photonic crystal cavity. Ion-beam milling was then used to define the photonic crystal. A silver tapered waveguide was grown in the centre of the cavity using electron beam induced deposition from a gas precursor containing a platinum–carbon polymer. A thin film of silver was deposited on the surface of the device (30 nm thick), and then silver removed locally from the photonic crystal surface. Finally, the sample was immersed in diluted fluoride acid for a few seconds to remove a 10-nm layer of silicon nitride implanted by gallium during the milling process.

The AFM IR-laser will be focused on the PC fabricated on the back of the cantilever, while the Raman signal will be collected from a high N.A. optics mounted on an inverted optical microscope. Additional geometrical configuration will be possible by collecting the optical signal by means of optical fibers. The signal will be analysed by a monochromator-CCD system (Fig. 2). The major advantages of the present device are that the nano-waveguide provides a considerable SPP enhancement, and that the excitation source (focused on the PC cavity) is spatially separated from the Raman active site. This decreases the perturbation effects of the source, the background signal, and provides increased sensitivity down to few-molecules detection.

Raman scattering and AFM measurements were performed with different substrate and experimental conditions; in particular the Raman spectrum of a silicon nanocrystal stripe on silica substrate is reported in figure 3. When a scan is performed across a stripe of silicon a clear variation of Raman signal (from silicon peak at 520 cm^{-1} to silica peak at 460 cm^{-1} can be observed. The corresponding AFM topography is reported in figure 4. In our best condition a chemical resolution of 7 nm is reached, also when Raman scattering and AFM topography are performed at the same time.

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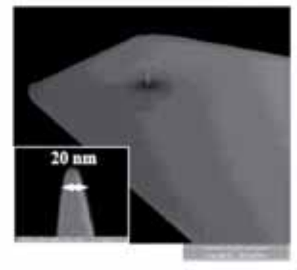

Figure 1. SEM image of the PC on silicon nitride cantilever with the silver cone acting as nanoantenna in the centre of the cavity.

Figure 2. Sketch of the experimental set-up, showing the integration of of the photonic –plasmonic device into an AFM-Raman microscope

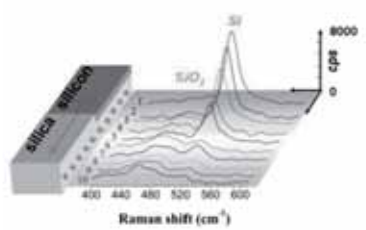

Figure 3. Raman spectrum measured across a stripe of silicon nanocrystal (figure 4). A clear variation of Raman signal can be observed when substrate change from silcon (520 cm-1) to silica (460 cm-1).

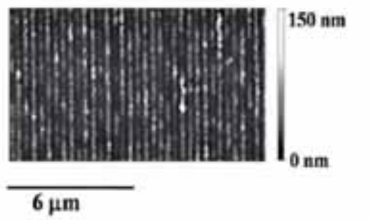

Figure 4. AFM topography of silicon nanocrystal stripe growth on silica substrate. The Raman spectrum performed across a single stripe is reported in figure 3.

Kissing spheres: broadband response and superfocusing properties

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One of the main limitations of plasmonic structures for light harvesting purposes is their narrow spectral response. In this work, we describe how geometrical singularities can be employed to overcome this apparent restriction. Following a similar strategy to that employed recently in 2D systems, we use analytical approaches based in transformation optics to study the scattering properties of a plasmonic dimer composed by two metallic spheres in contact at a single point. We demonstrate that these *kissing spheres* exhibit a broadband response, leading to an efficient far to near field transfer of electromagnetic energy at frequencies well below the metal plasma frequency. We will also show that this effect is accompanied by the occurrence of an enormous field enhancement close to the touching point, where the incoming electromagnetic energy accumulates. Finally, by means of numerical simulations, we explore the range of validity of our analytical results and discuss the potential applications of kissing spheres as highly efficient electromagnetic scatterers.

Active magnetoplasmonics in hybrid metal/ferromagnet/metal microinterferometers

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Surface plasmons polaritons (SPP) are evanescent waves that propagate along a dielectric-metal interface. They can be confined in subwavelength metal structures, i.e. below the diffraction limit, which leads to many possible applications, including miniaturized optical devices. Within that context, the development of active plasmonics is important to achieve nanophotonic devices with advanced functionalities. This requires a system where the plasmon properties can be manipulated using an external agent. Among the different control agents considered so far, the magnetic field seems a promising candidate, since it is able to modify the dispersion relation of SPP at reasonable magnetic field strengths, and with a high switching speed. This modulation comes from the non-diagonal elements of the dielectric tensor, ϵ_{ij}, appearing when the magnetic field is turned on. For noble metals, the ones typically used in plasmonics, these elements are proportional to the applied magnetic field but, unfortunately, very small at field values reasonable for developing applications. On the other hand, ferromagnetic metals have sizeable ϵ_{ij} values at small magnetic fields (proportional to their magnetization), but are optically too absorbent. A smart system to develop magnetic field tunable plasmonic devices is the use of multilayers of noble and ferromagnetic metals.

In this work, we analyze the magnetic field induced SPP wavevector modulation in Au/Co/Au films by means of surface plasmon interferometry. We study its dependence on the position of the Co layer and on the wavelength. We will show that we can obtain modulation values of the order 1×10^{-3}. The are several ways to further improve this modulation, among them we will briefly discuss the effect of covering the Au/Co/Au trilayer with a dielectric medium with high ϵ_d. We have measured a fourfold increase of the SPP wavevector modulation when coating our samples with a thin layer of PMMA.

Collective plasmonic resonances in arrays of nanoantennas

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Metallic nanoparticles supporting surface plasmon resonances allow the localization of electromagnetic fields in nanoscale volumes. This unprecedented localization of light has opened exciting possibilities, such as nanoscale control of emitters, large electromagnetic enhancements, and non-linear nanoscale optics.

A new development in nanoplasmonics deals with the enhanced radiative coupling of localized surface plasmon resonaces in periodic arrays of nanoantennas, which leads collective resonances known as surface lattice resonances. This coupling is mediated by Rayleigh anomalies or diffracted orders grazing to the surface of the array. The hybrid plasmonic-photonic character of surface lattice resonances gives rise to giant field enhancements and very sharp resonances in the extinction spectra of the array, with Q-factors more than one order of magnitude larger than the Q-factors associated to localized surface plasmon resonances.

In this contribution we discuss new experimental aspects of surface lattice resonances such as diffractive coupling of multipolar resonances, modified emission of light emitters in the proximity of arrays of nanoantennas and strong coupling of surface lattice resonances.

Self-induced back-action optical trapping

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Optical trapping has widely affected both the physical and life sciences. Past approaches to optical trapping of nanoscale objects required large optical intensities, often above their damage threshold. To achieve more than an order of magnitude reduction in the local intensity required for optical trapping, we present a self-induced back-action (SIBA) optical trap, where the trapped object has an active role in enhancing the restoring force. We demonstrate experimentally trapping of single 100 and 50 nm polystyrene spheres (figure 1) using a SIBA optical trap on the basis of the transmission resonance of a nanoaperture in a metal film Ref. [1]. SIBA optical trapping shows a striking departure from previous approaches, which we quantify by comprehensive calculations.

While the initial design consists of an aperture in an extended gold film, we show that the SIBA approach has been successfully transposed to a mobile scanning probe. This new approach, allying a robust and low intensity trapping to the ultra accurate positioning of the probe, constitute a promising new platform for the manipulation of nanometric dielectric objects.

In this context, the SIBA optical trap enables new opportunities for non-invasive immobilization and manipulation of a single nanoscale object, such as a virus or a quantum dot.

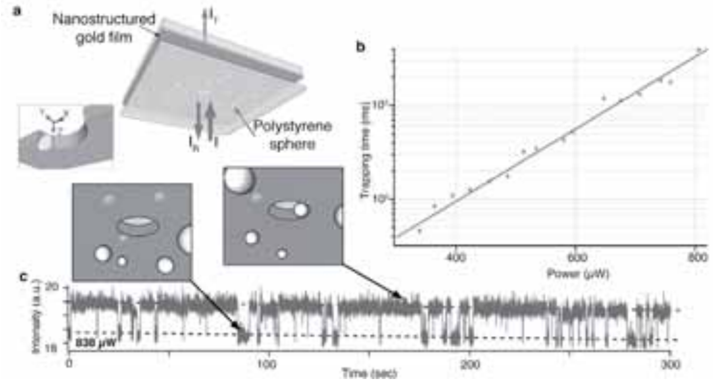

Figure1: Experimental trapping of 100 nm polystyrene spheres. (a) schematic view of the experimental setup where I, I_T, and I_R are the incident, transmitted and reflected intensities respectively. (b) experimental trapping time dependence with the incident laser power. (c) experimental time evolution of the transmitted intensity with 0.838mW of laser power. The high and low values of the transmission constitute a direct signature of the presence of a sphere in the aperture.

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Plasmonic control of elementary emitters

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Surface plasmons are electromagnetic modes at the interface of a metal and a dielectric that can be focused to nanoscale volumes and that feature resonantly enhanced near fields. Coupling plasmonic modes to elementary emitters as molecules or semiconductor nanocrystals is of specific interest, as this coupling can strongly alter both, the excitation and emission rates of the emitters. Here, we focus on the emission process that is governed by the photonic local density of states. This quantity can be tailored by controlling the geometry-dependent resonance frequencies of plasmonic nanostructures by lithographic means. On this basis we report emission rate engineering of fluorophores [1], redirecting the energy flow in molecular resonance energy transfer [2] and refined insight in surface enhanced Raman scattering [3]. For better controlling the mutual position of plasmonic nanoparticles and molecules we have developed a lithographic method that combines metal nanoparticles with molecule-doped polymer nanoparticles. We demonstrate that their mutual position can be controlled to within a few nm by imaging the local density of states of the plasmonic particles by Moire patterns generated by combining incommensurable regular arrays of both types of nanoparticles [4].

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Extraordinary optical transmission due to strongly localized modes

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Extraordinary optical transmission (EOT), i.e, the phenomenon in which a set subwavelength apertures in an opaque screen transmit more light than what directly impinges on them [1], has attracted a great deal of attention due both to its fundamental interest and potential applications[2].

Two main mechanisms leading to EOT has been unveiled: transmission aided by electromagnetic surface modes and through localized resonances. While in the first case, the spectral positions at which the transmission resonances occur are well analyzed, the second case has been less studied.

In this talk we show how the characteristics (peak position and peak height) of the localized transmission resonances depend on both metal thickness and dielectric substrate, in the THz regime. We show that the transmittance is governed by the cutoff wavelength of the hole and an additional length scale, related to who the hole "feels" the radiation regions.

Some numerical results will be presented in the optical regime, showing that the transmittance aided by localized modes presents the same overall dependence with metal thickness as in the THz.

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Improving the efficiency of luminiscent solar concentrators

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The basic idea behind luminescent solar concentrators (LSC) is to concentrate sunlight with an inexpensive device and thus reduce the price of solar electricity. An LSC consists of a glass or plastic plate coated with dyes that absorb sunlight and emit light at longer wavelengths. A substantial part of the longer-wavelength light is trapped by total internal reflection and guided to the edges of the LSC plate, where it is absorbed by small-area PV cells. Advantages over geometric concentrators include that expensive solar tracking is unnecessary and that both direct and diffuse radiation can be collected.

LSC was suggested in the late 1970s. However, the development of this promising concentrator was limited by factors like the performance of the luminescent dyes, the poor stability of the dyes under solar irradiation, the large re-absorption losses owing to significant overlap of the absorption and emission and the isotropic emission of the radiation. In this communication, we will address recent developments in order to avoid these problems and improve the efficiency of LSCs.

Acknowledgments
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Electromagnetic interaction between plasmoned nanostructures and substrates

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The sensitivity of localized plasmon resonances (LPR's), excited in metallic nanostructures, to the optical properties of their environment, has opened new possibilities for surface monitoring and then opening doors to new techniques in optical microscopy based on plasmonics [1]. The electromagnetic interaction between a nanoprobe, where a LPR is excited, and a sample substrate, produces variations in the spectral response of the LPR (shift and broadening) whose detection can provide with information about the optical characteristics of the substrate. In this contribution, we present a numerical analysis, based on DDA (Discrete Dipole Approximation) [2], of the Physics involved in the interaction between a metallic nanoprobe and the surface underneath. Different scattering configurations will be considered. The sensitivity for observing local changes in either the optical constants or the geometrical profile of the substrate is analyzed by detecting the spectral changes in either intensity [3] or polarization of the scattered radiation. For the latter, a convenient parameter is the spectral linear polarization degree of the scattering at right angle configuration [4]. Finally, it is worth noting that other systems of growing interest are also considered, like flat substrates constituted by several thin layers of different dielectric constants.

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Theory | 10:30 | 01 SEPT.

Active plasmonic nanoantennas for optical switching

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We present a novel concept of ultrafast optical switches based on nonlinear plasmonic nanoantennas. Linear optical and infrared nanoantennas are capable to tune the electromagnetic response by impedance loading of its nanogap using a dielectric or metallic medium [1]. In this work we explore the use of a photoconductive load at the antenna gap to act as an effective optical nanoswitch [2]. The principle of switching is based on the transition from capacitive to conductive coupling between two plasmon modes when bringing two nanoparticles into physical contact. We show that photoexcited free carriers in a semiconductor material can be used as a load to short circuit the antenna arms, leading to a strong modification of both the spectral resonance structure and near-field mode-profile. As the plasmonic antenna switch is based on a strong confinement of optical fields in space rather than in time, the nanoantenna switch can operate at very low switching energy while potentially reaching a much faster response than microphotonic switching devices. We will present the theoretical concept as well as the first steps toward experimental realization of plasmonic nanoantenna switches.

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Interactions of excitons with localized surface plasmons in organic semiconductor-metal nanoparticle thin-films

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Localized surface plasmon resonances (LSPRs) excited in metal nanoparticles are receiving a large amount of attention recently as they are highly sensitive to the nanoparticle material, shape, size, and the dielectric environment, making the them tunable within almost any frequency in the IR, VIS or UV spectrum. Furthermore, they can lead to a strongly enhanced electromagnetic field near the metal nanoparticles. These features give metal nanoparticles potential applications in sensors, photovoltaic cells, light emitting devices, and surface-enhanced Raman scattering spectroscopy.

When metal nanoparticles are embedded in a light absorbing organic medium, the LSPRs interact with the excitons generated in the organic medium. In order to characterize these interactions, we measured the light absorption and photoluminescence of thin-films consisting of silver nanoparticles and small-molecule organic semiconductors. The organic semiconductors chosen for these experiments, copper phthalocyanine (CuPc) and chloroboron subphthalocyanine (SubPc), were chosen due to their use in organic solar cells. Thin-films with and without spacer layers between the nanoparticles and the organic semiconductor were examined.

We observed an increase in light absorption of CuPc and SubPc in presence of Ag nanoparticles. Moreover, in the case of SubPc, the excitation of an additional dipole LSPR was observed due to its highly dispersive permittivity. These experimental results are in good agreement with finite element simulations. The photoluminescence of SubPc was reduced by almost a factor of two in the presence of the Ag nanoparticles without a spacer layer, but increased by a factor of 1.4 when a spacer with a thickness below 5 nm was introduced.

Moving plasmonic nanoparticles through electromagnetic forces induced by fast electron beams

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Recently, has been observed experimentally the dynamics produced on gold nanoparticles supported on amorphous carbon by fast electron beams, like those used in last generation aberration-corrected scanning transmission electron microscopy (STEM).

The motion induced on nanoparticles system yields to a coalescence phenomenon, when the sizes of the nanoparticles interacting with the electron beam are larger than ~1 nanometer. One can regard the fast electrons as a broad frequency range of electromagnetic fields probing the plasmonic nanoparticles, which couple with the metallic particles by means of inducing surface charge densities and transferring mechanical momentum to them. This momentum transfer depends on the impact parameter of the beam, the size of the nanoparticle, and the dielectric response of the material.

In this contribution, we calculate the momentum transferred by fast electron beams to a pair of metallic particles (aluminium and gold dimers), by integrating the electromagnetic forces acting on the particles over time (or equivalently by integrating over frequency).

We show that depending on the specific values of the parameters as impact parameter of the beam, size of the nanoparicle and dielectric response of materials involved, the total momentum transfer yields a force that can be either attractive or repulsive. Furthermore, we also show that the electromagnetic forces induced on metallic nanoparticles by fast passing electrons are comparable in magnitude to the optical forces, thus suitable of moving and changing the configuration of particles observed under transmission electron microscopes.

30 SEPT. | 10:50 | Electrons and Photons

A scanning tunneling microscope as a tunable nanoantenna for atomic scale control of optical-field enhancement

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The controllable enhancement of a confined optical-field at the nanoscale opens a wide range of applications including single element detection, near-field nano-imaging or photochemistry [1-3]. While the issue of the sole confinement is successfully solved via the concept of nanoantennas, the simultaneous tuning and monitoring of the optical-field enhancement is still a defying objective[4]. Here, we exploit the stability of a low temperature (9K) scanning tunneling microscope (LT-STM) junction to precisely adjust the enhancement of an external pulsed vacuum ultraviolet (VUV) laser. The ensuing VUV optical-field strength is mapped on an hydrogenated Si(100) surface used as a photo-resist to reveal one-photon atomic scale hydrogen desorption. Subsequent topography of the Si(100):H surface at the reacted area points-out desorption spot with unprecedented atomic precision. Our results show that their shape, positions and sizes are precisely correlated to the calculated optical-field structure, offering a real control of the optical-field distribution at molecular scale.

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LDOS fluctuations probed by single-molecule spectroscopy in random and periodic media

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We report on measurements of fluorescence lifetime of point-like sources in complex dielectric media. The large spatial fluctuation reveals the spatial variation of the local density of states of the nanostructured media.

Large spatial fluctuations of the LDOS in random media has been theoretically predicted and linked to both the C_0 intensity correlation function and to the scattering mean free path [1]. The central role of the LDOS has also been highlighted in the context of periodic media [2], and has been the topic of many further investigations. Very recent experiments for diamond N-V centers [2] and polymer beads [3] in disordered dielectric matrices have given a clear indication of enhanced lifetime fluctuations.

In this work single Alexa Fluor molecules and dye-doped fluorescent beads (20nm diameter), have been introduced in macroscopic arrangements of dielectric particles, both periodic in the form of direct polystyrene (PS) and inverse ZnO opals, and random as compact dielectric powders.

Confocal microscopy and time-correlated single-photon measurements allow for addressing individual sources buried as deep as 10-20 micron inside the nanostructured matrix, with a time resolution below ~100 ps. Two typical intensity images are plotted in fig 1., for a random and ordered matrix.

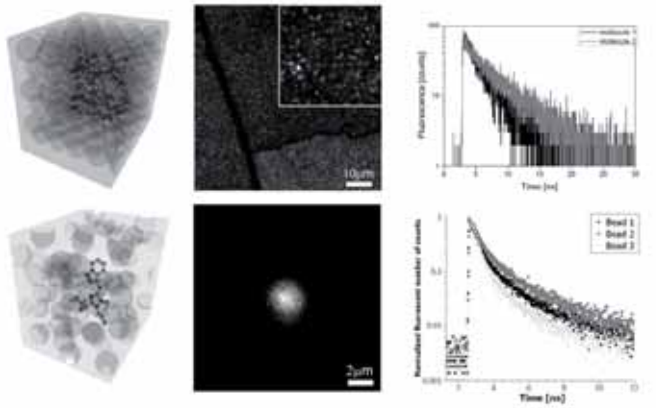

Fig. 1 Geometry sketch, fluorescence confocal images and lifetime traces of single molecules in a direct PS photonic crystal (top panels) and one dye-doped bead in a ZnO powders, (bottom panels).

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Nanoplasmonics by Protein Technology

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Controlling the surface binding, distribution, and targeting of nanoparticles is a key element to realise nanoplasmonics devices. For this, self-assembly is a very attractive technique. Because self-assembly is essential to biology at the molecular scale, it is interesting to turn to biology for inspiration and tools for nanofabrication. Advantages of biomolecules include the highly selective and specific interactions. Proteins additionally have the advantage that their structure is highly defined and that techniques are available for very precise engineering. In order to control structures over orders of magnitude in dimensions and hierarchy, an interesting aim is to combine top-down and self-assembly techniques for directed self-assembly. This work presents new tools for building devices for nanoplasmonics by utilising a selectively binding protein, hydrophobin [1]. The proteins form ordered 2-dimensional semi-insulating surfaces on top of hydrophobic materials. The materials include silicon, graphite, graphene and polystyrene, among others. The protein layer is one monolayer, about 2 nm, thick, and has a hexagonal lateral lattice with a lattice constant of about 6 nm. Hydrophobins modified by genetic engineering to display a single reactive -SH group to bind gold nanoparticles were used in the experiments. By first depositing a monolayer of hydrophobins on a solid surface, gold nanoparticles can be bound to the surface. UV-vis spectra of NCys-hydrophobin - modified glass slides exposed to the nanoparticle solutions were measured. The gold nanoparticles attached to the surface without precipitating. At longer incubation time plasmon coupling band appeared, showing interaction between the nanoparticles. TEM images show no clustering of the Au particles. In this work we have shown that biotechnology can be used in fabrication of plasmonic structures utilising the directed self-assembly of engineered proteins.

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Near field study of Silicon micro-nano structures in the near infrared

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Plasmonic based subwavelength optics and its applications, such as the synthesis of negative-index optical materials (metamaterials) together with the design of optical antennas have been subject of great interest in the nano-optics field during the last decade. So far, most of the experiments searching for magnetic plasmons and magnetic resonant structures at optical frequencies have been mainly focused on metallic structures, leaving dielectric materials apart. However, as an alternative approach, there is a growing interest in the theoretical and experimental study of high-permittivity dielectric objects as constitutive elements of new metamaterials and antennas based on dielectric resonators.

Motivated by the interesting magnetodielectric properties of certain low loss and large dielectric constant materials (Si for example) we analyze in detail the near field of Si structures grown on substrates, paying special attention to the relevance of the different magnetic resonances in low-absorbing dielectric structures (e.g. silicon interacting or isolated cubes in the near-IR regime). A variety of near-field patterns can be induced at different wavelengths in micron-sized Si structures. We identify these patterns and connect them with the electric and magnetic activity at the sample. Our results provide an understanding of optical experiments performed on this substrates.

29 SEPT. | 15:00 | Poster Session

Dynamics of spinning particles under external illumination

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We study the rotational dynamics of illuminated nanoparticles. Analytical expressions are obtained for the electromagnetic torque, absorbed power and light scattering cross sections. A non-trivial dependence of these quantities on the rotation velocity is obtained, accompanied by emission of light at frequencies shifted with respect to the incident light by twice the rotation frequency, depending on the external light polarization.

The dynamics of such particle is analyzed under extreme rotation conditions. At sufficiently large rotation velocities, the particle is deformed by centrifugal forces and it eventually splits into fragments. Our results sugest new possibilities for exploring the mechanical properties of nanoparticles.

Plasmon-enhanced photoemission from a single rare-earth fullerene

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Rare earth ions are a crucial component in modern optoelectronic devices.
However, optical experiments at the single-ion level are elusive because of low absorption strengths and long excited-state lifetimes.
Using a gold nanoparticle as a plasmonic antenna, we have performed the first single-molecule photoemission study of an endohedral metallofullerene. This molecule consists of 3 yttrium and 1 nitrogen ions encapsulated inside a C80 fullerene cage (Y3N@C80).

The effect of the antenna is two-fold: it increases light absorption by the yttrium cluster, and also aids light emission by increasing the radiative decay rate of the molecule. Overall, this leads to huge enhancements in photoluminescence of 2 orders of magnitude, making the antenna-coupled yttrium nitride fullerene as efficient as an ordinary dye molecule. Our results have implications for improving the performance of low efficiency systems like nanocrystalline silicon and organic semiconductors.

29 SEPT. | 15:00 | Poster Session

Plasmonically Modified Resonance Energy Transfer

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Förster resonance energy transfer (FRET) is a process where an excited fluorophore (the donor) excites a nearby ground-state fluorophore (the acceptor). The non-linear efficiency of this process is characterized by the Förster radius, R_0, and enables a nanometer resolution of intermolecular spacing. FRET is an established method in biochemistry and cellular biology. However, the Förster radius is typically only a few nanometers, limiting the potential of FRET in many applications.

The influence of plasmonically active particles in the vicinity of fluorophores on their optical properties have been studied both theoretically[1] and experimentally[2]. As for FRET, the influence of films3 and particles have been investigated[4, 5]. However, there are still many open questions regarding the possibility to modify FRET using plasmonic nanostructures.

In this study we will present results based on DNA-functionalized nanoparticles fabricated using EBL. The DNA enables the positioning of fluorophores with Angstrom resolution and EBL fabrication makes it possible to study a variety of nanoparticle shapes and sizes. In addition, we are theoretically investigating FRET in the vicinity of nanoparticles using extended Mie theory. We hope that the current work will be of importance both for the biologic community and for nanophotonic applications, such as solar cell development.

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Poster Session | 15:00 | 29 SEPT.

Coherent Control of Femtosecond Field Dynamics around Nanoantennas

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Nano-antennas can be used to couple near field phenomena to far field excitation at optical frequencies, in analogy with classical radio wave antennas [1]. They concentrate electromagnetic fields in sub-diffraction limited hotspots [2], whose position in time and space depends on the antenna-structure and the incoming electromagnetic field [3]. Antennas can therefore be combined with ultrafast pulses to address femtosecond processes in nanometric volumes. To achieve this, one needs to adapt the properties of the incoming field to the dispersion of the antenna-structures [4].

We adjust the field of an excitation pulse to the dispersion and resonances of an optical gap-antenna and map the resulting changes in field enhancement in the hotspots. Asymmetric gold nano-antennas are lithographically fabricated with high reproducibility. Experiments are conducted on matrices of parametrically differentiated (length, gap position) structures to ensure identical excitation conditions for each antenna. The local field around a nano-antenna, resulting from excitation with a phaseshaped femtosecond pulse, is resolved with Two Photon Luminescence (TPL) [5].

Using the two photon signal of the antennas for differently phase shaped excitation fields, a signature of the local phase along the antenna is obtained, proving the possibility of phase-engineering by controlling the coupling between nanostructures.

Pure phaseshaping is used to steer hotspots to different positions within one nanoantenna on a femtosecond timescale. Resolving this movement in a pump-probe experiment gives quantitative information about the femtosecond field dynamics around the structure.

Our latest experimental results will be presented and discussed in the context of implementing nano-antennas in molecular coherent control experiments.

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29 SEPT. | 15:00 | Poster Session

Polarized multiphoton emission from resonant Al, Ag and Au nanoantennas

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Optical antennas have gained major importance as coupling elements between near and far field in nanoscale photonics [1]. Although nanoantennas are already widely being used [2, 3], their fabrication and characterization are still challenging and no systematic experimental comparison between antennas of different metals has been made.

We present an experimental study of optical rod antennas of three different metals: Aluminum, Silver and Gold. We identify the first (lambda/2) and third (3lambda/2) resonance modes by two-photon luminescence (TPL) analysis [4] and the relative shift between the metals due to their different plasmon characteristics. Whereas plasmonic studies are usually performed on gold, here we show that Al [5] is a suitable metal for the fabrication of optical antennas due to its strong TPL response.

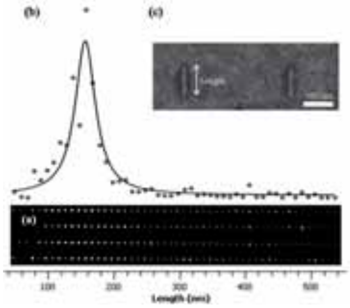

Figure 1. Measuring TPL resonance of aluminum nanoantennas.
(a) TPL image of four identical rows of aluminum rod nanoantennas with increasing lengths between 50 nm (left) and 540 nm (right). (b) TPL intensity profile averaged over the four rows of nanoantennas. The structures exhibit a clear resonance upon excitation with a 14 fs pulse at central wavelength 780 nm. (c) SEM image of two consecutive aluminum rod antennas of 500 (left) and 510 nm (right) lengths respectively.

Interestingly, a polarization analysis gives new insights into the nature of optical resonances of nanostructures. When the polarization of the incident light is along the rod, the antennas are excited very efficiently giving high intensity luminescence. We see that this TPL signal is unpolarized in the case of gold, while aluminum strongly follows the polarization of the excitation. This shows that aluminum preserves the polarization of the antenna modes much better than gold, where the contribution of the transversal mode rivals with the longitudinal one resulting in an unpolarized luminescence.

On the other hand, when the polarization of the incident light is orthogonal (perpendicular to the rod) the TPL signal drops to almost zero for aluminum and silver. The transversal mode is still present on gold although the antenna is inefficiently excited thus the luminescence intensity also drops considerably.

In conclusion, a systematic approach shows a surprisingly good performance of Al antennas in both linear and non-linear response. Better understanding of the role of different metals will lead to more efficient designs for nanooptical elements and plasmonic structures.

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Phase-Sensitive Near-field Imaging of Optical Nano-antennas

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Antenna theory has been well established and applied for hundred years in radiowave technology. Current technological capabilities have achieved nanoantenna structures down to the nanoscale, boosting extensive studies on potential nanoantenna applications ranging from nanoscale photodetectors [1] to highly sensitive biosensors [2]. Many of the applications rely on the near-field performance of the nanoantenna. In this poster we report phase-sensitive near-field imaging of nano-antenna modes in the visible spectral range (632.8nm excitation). Near-field probing is performed with a dielectric silicon AFM tip and pseudo-heterodyne interferometric detection [3]. Polarization-resolved mapping of nanoscale vector fields is performed by an orthogonal excitation and detection scheme [4], where the polarization of incoming laser is oriented parallel to the nano-antenna axis (s-polarization). A linear polarizer is placed in front of detector to selectively detect amplitude and phase of the out-of-plane (vertical) component of the antenna near fields. The use of sharp Si tips allows for mapping even the strongly confined near fields in and around nanoscale antenna gaps.

We will present near-field amplitude and phase images of resonant gap antennas, directly visualizing the field confinement in the antenna gaps. We will also show that the phase images of the vertical field component can be related to the surface charge distribution.

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Detection of Disease Specific Enzymes Using Surface Enhanced Raman Scattering (SERS)

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Certain enzymes act as distinctive biomarkers for specific diseases the detection of which at low concentrations is critically important for healthcare diagnostics.

Although a number of methods for the detection of such enzymes exist little is known or understood about enzyme dynamics. Moreover the study of enzyme interactions at ultra-low concentrations is typically quite demanding.

In recent years surface enhanced Raman scattering (SERS) has generated a great deal of interest due to its sensitivity and molecular specificity.

However, all proposed applications of SERS to date have ignored hotspots due to a lack of reproducibility.

Recently nano-particle assemblies have been created through the functionalization of gold nanoparticles with a short peptide chain terminated by an FMOC molecule which is specific to a particular enzyme.[1]

These self-assemble into aggregates due to π-π; interactions allowing close and reproducible control of the plasmonic properties.

Upon addition of the enzyme, the peptide is cleaved causing the disintegration of the nano-particle assemblies. This process could in principle allow for the SERS hotspot to be used reliably for the first time.

The purpose of this present work was to determine if SERS would offer any potential advantage over the prior methods for enzyme detection.

Our results suggest that the technique may offer extraordinary sensitivity and that the presence of the enzyme can be reliably detected over a wide range of concentrations relevant to medical diagnostics [4].

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In-Situ Raman Spectroscopy of Graphene in Reducing Atmospheres

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The unique electrical and mechanical properties of graphene make it attractive for a wide range of applications including chemical sensors, transparent flexible electrodes and high performance interconnects in integrated circuits. Typically the highest quality graphene has been produced through the mechanical exfoliation of graphite, a process characterized by a low yield of extremely high quality flakes. Although the method is suitable for research purposes, the low yield makes it unsuitable as a source for practical applications. A number of alternative methods for the high yield production of graphene at have been developed including wafer scale annealing of Silicon carbon, reduction of graphene oxide, exfoliation of graphite in solution and chemical vapor deposition. These methods are typically high yield, compatible with existing fabrication techniques and, in the case of graphene oxide and exfoliated graphite, solution processable. While such methods allow for the large scale production of graphene, the quality of the films is generally lower than that obtained through the mechanical exfoliation. Raman spectroscopy is a particularly powerful characterization tool for carbon species and has a rich history in similar low dimensional carbon system such as carbon nanotubes. The clear Raman fingerprint of carbon allows for the investigation of defects, doping and electronic structure with clear differences observed for graphene of different number of layers. In this work we investigate in-situ Raman annealing of graphene prepared using different methods in reducing atmospheres.

29 SEPT. | 15:00 | Poster Session

Spatial Dispersion in the Optical Response of Metallic Nanoparticles using Advanced Material Models

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Spatial nonlocality is known to play an important role at distances of a few nanometers, but few efforts have been made to theoretically investigate nonlocal effects in a rigorous way. We present two different approaches to account for nonlocality in metal nanoparticles: (a) the non-retarded specular reflection model (SRM) and (b) the retarded hydrodynamical model. Comparison with available experiments results in excellent agreement with our parameter-free modeling of nonlocal effects, which produce dramatic changes with respect to the customary local theory. We show that nonlocal effects in both models produce sizable plasmon blue shift and broadening in single metal nanoparticles as well as in dimers and nanoshells. Analysis of the plasmon resonance dependence for dimers on the inter-particle spacing and nanoparticle size allows us to separate nonlocal and retardation effects within the hydrodynamical model. This study is particularly relevant for broad, active areas involving applications of local field enhancement to biosensing and nonlinear optics.

A highly reproducible SERS detection of biomolecules using lithographied Nanoparticles: application to biosensor

DAVID Catalina[1], GUILLOT Nicolas[1], SHEN Hong[2], TOURY Timothée[2], LAMY DE LA CHAPELLE Marc[1]

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The purpose of the present study is to achieve a SERS sensor with extreme sensitivity and very high molecular specificity by combining the enhancement of vibrational signal, surface functionalization, respectively, and detection of vibrational Raman spectra signals in order to provide at very low concentration the spectral signature of proteins. Our SERS sensor is based on gold nanocylinder arrays obtained by Electron Beam lithography. The preliminary results concern the first study of SERS efficiency of nanocylinder arrays at 632 nm in the case of proteins, BSA and RNAse. The maximum SERS intensity obtained for a specific nanocylinder diameter.

29 SEPT. | 15:00 | Poster Session

Optimizing the excitation of gap cavity modes by linear antenna modes

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Classical linear antennas formed by thin rods support resonant modes along the rod axes. For two rods at short distance and optical frequencies, modes of a different nature can appear in the gap. These are cavity modes propagating perpendicularly to the axis. We use the boundary element method (BEM) to solve the classical Maxwell equations and study the intriguing interplay between both families of modes.

We consider simple rotationally simmetric rods described by a drude metal. The far field results are mostly dominated by the antenna modes, with a clear dipolar resonance and weaker signatures from resonances of higher order. The behavior of the near field enhancement is however significantly more complex, with a large multiplicity of peaks for distances smaller than approx. 1nm. These peaks can be associated with the excitation of gap cavity modes of different orders, but they are not completely independent of the linear antenna modes. Notably, the near field enhancement achievable is a function of the excitation strength of both modes. We obtain enhancements of the electric field of almost 500 by efficiently exciting both a cavity and a linear antenna mode at the same wavelength.

We also notice that the maximum position of the far field peaks redshifts with decreasing distances, but the shift saturates for values going to zero. Intriguingly, this differs markedly from the observed behavior for spheres, where the shift increases fast for short distances. We believe that the qualitative difference is connected with the interplay between the modes in our structure, an aspect we are studying. We are also interested in the behavior for real metals and the effect of quantum effects, which should be important at the smallest considered distances.

Engineering the Near-Field of Metallic Nanoantennas: Enhancing Possibilities in Spectroscopy and Microscopy

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Optical antennas are nanoscale metallic structures which act as effective receivers and transmitters of visible and infrared (IR) light. These nanoantennas show the ability to focus electromagnetic radiation into tiny spots of nanometer scale dimensions allowing for field-enhanced nano optical applications. We adress here the basic ingredients that allow optical nanoantennas to perform very effectively in enhanced spectroscopy and microscopy. We show how to engineer these ingredients through the manipulation of the geometry and coupling in the antenna configurations, maximizing their near-field and tuning the spectral response for a particular application in visible or infrared (IR) spectroscopy and microscopy.

Engineering the length of a rod-like nanoantenna, for example, it is possible to tune the resonance of the antenna to the IR part of the spectrum and perform direct surface-enhanced infrared absorption (SEIRA) of a few molecules on a single nanoantenna. With use of this concept, we show how it is possible to enhance the signal and contrast of the molecular fingerprints of organic groups deposited on the antenna.

Another option to engineer the optical response of a nanoantenna relies on the manipulation of the antenna gap. We show theoretically and experimentally the modication of the optical response of nanoantennas as a function of the thickness of the antenna gap, bridging together concepts of optics and circuit theory.

The interaction between tip and sample in scattering-type near field optical microscopy (s-SNOM) can also be understood as an antenna-antenna interaction effect. Under convenient conditions of light incidence, polarization scheme and tip characteristics, the near-field interaction allows for direct mapping of near-field patterns with nanoscale resolution in a wide spectral range from the visible to the Terahertz. A theoretical description of the interaction process is presented and two different interaction regimes are identified: (i) strong and (ii) weak interaction regime.

From the overview and the examples shown here, we conclude that an understanding of the interactions occurring at the nanoantennas and the knowdledge of the electromagnetic response in different configurations are crucial to engineer and design plasmonic devices showing properties on demand.

29 SEPT. | 15:00 | Poster Session

III/V Solar Cells with a Multi-Functional Plasmonic Light Concentration Layer

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Conversion of solar energy into electricity is considered one of the most promising solutions to the energy problem. Conventional III-V solar cells are designed such that their optical depth for absorption relates directly to the thickness of the absorbing material. This results in relatively thick solar cell structures consuming valuable semiconductor material and increasing the solar cell manufacturing time[1]. The ability to manipulate light using plasmonics could be extremely advantageous, enabling the optical depth for absorption becomes much greater than the thickness of the absorber, resulting in enhanced light absorption in thin-film solar cells[1, 2].

We investigate theoretically and numerically the interaction of light with periodic arrays of metal nanoparticles on thin film of GaAs (~100nm). Our purpose is to enhance the light absorption in solar cells by employing excitation of localized surface plasmon resonances (SPR), grazing diffracted orders and light coupling into guided modes in the GaAs thin-film.

In this contribution we demonstrate that the three methods can be employed at the same time in the same structure obtaining a three-fold effect in the range where the GaAs is almost transparent.
Thin-films of GaAs in optimized structures following that idea can absorb up to 5 times more than a bare structure without metal nanoparticle.

Such a configuration is specially relevant because does not affect to the absorption already high at shorter wavelengths (300nm-700nm) and strongly improve the absorption at longer wavelengths.

References

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2 K. R. Catchpole et al., Optics Express 16, 21793, (2008).

Optical interactions on small magnetodielectric particles

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We present a study of the optical force on a small particle with both electric and magnetic response, immersed in an arbitrary non-dissipative medium, due to a generic incident electromagnetic field. This permits us to establish conclusions for any sign of this medium refractive index. From the formal analogy between the conservation of momentum and the optical theorem, we discuss the origin and significance of the electric-magnetic dipolar interaction force; this is done in connection with that of the angular distribution of scattered light and of the extinction cross section. We explain the electric-magnetic dipolar interaction term of the force in analogy with the contribution of the interference between the fields radiated by the electric and magnetic dipoles to the angular distribution of scattered intensity, or differential scattering cross section, in comparison with that of the total scattering and extinction cross sections.

Further, we obtain expressions for the gradient force, radiation pressure and curl components for the force due to both the electric and magnetic dipoles excited in the particle. In particular, for the magnetic force we tentatively introduce the concept of curl of the spin angular momentum density of the magnetic field, in analogy to pure electric dipole forces. In this form, we derive a non-conservative contribution of the magnetic term as proportional to the curl of a tentatively introduced spin angular momentum density of the magnetic field. Also, the electric/magnetic dipolar interaction component contributes to both the radiation pressure and gradient forces. These results show the complementary contribution of the electric and magnetic fields to these forces, depending on the polarization. This opens the way to future research on some composite metallic or dielectric particles of high refractive index that should present substantial response to the magnetic field of an electromagnetic wave in the infrared and visible regions.

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29 SEPT. | 15:00 | Poster Session

Surface Enhanced Raman Scattering of gold nanostructures: Role of dipolar and multipolar localized surface plasmons

GUILLOT Nicolas[1], FREMAUX Benoît[1], BEN AMOR Salem[1], SHEN Hong[2], PERON Olivier[3], TOURY Timothée[2], IFREMER Emmanuel[3], LAMY DE LA CHAPELLE Marc[1]

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We have studied the Surface-Enhanced Raman Scattering (SERS) of shape controlled metallic nanoparticles: nanocylinders and nanowires, designed through electron beam lithography and lift off techniques. We have notably studied the influence of Localized Surface Plasmon Resonance (LSPR) on the efficiency of SERS. We will demonstrate that the nanowires have specific enhancement behavior and can actually act as nano-antenna.

SERS Optimization Of Gold Nanocylinders Arrays: Influence Of The Surrounding Medium And Application For Polycyclic Aromatic Hydrocarbons Detection

GUILLOT Nicolas[1], SHEN Hong[2], BEN AMOR Salem[1], DAVID Catalina[1], PERON Olivier[3], RINNERT Emmanuel[3], TOURY Timothée[2], LAMY DE LA CHAPELLE Marc[1]

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This study describes the effect of the surrounding medium on the SERS efficiency using nanolithographied substrates on which Polycyclic Aromatic Hydrocarbons are investigated. We will show that the optimum nanocylinder size is shifted to lower diameter by increasing the dielectric constant of the liquid medium. This rule is discussed in terms of Localized Surface Plasmon Resonance since its position influences directly SERS intensity. This study is done for two excitation wavelengths: 632.8 nm and 785 nm. The aim of this work is collect information in order to product future active SERS sensors suitable for in situ environmental analysis.

29 SEPT. | 15:00 | Poster Session

Engineered plasmonic structures: Enhanced Raman scattering and stretch tunability

HUGALL James T[1], MAHAJAN Sumeet[1], HUANG Fumin[1], BAUMBERG Jeremy J.[1]

[1]NanoPhotonics Centre University of Cambridge, Cambridge, UK

Periodic nanostructured metallic surfaces are highly-effective light traps, where localised surface plasmons become confined and therefore enhance the electric field at locations within the nanostructures. This trapped electric field, with amplitude around 100 times that of the incident light, can be used to enhance many optical processes, including Raman scattering, fluorescence and even solar cell efficiency.

Here we focus on surface-enhanced Raman scattering (SERS) and demonstrate SERS of a sub-monolayer of QDs on both self-assembled hexagonal dish structured nanovoids, and commercially-available inverted pyramid structure, Klarite™ [1]. Further enhancement of SERS by resonance with the QD electronic transitions is shown to provide enhancements large enough for single QD detection. Investigation of the distance dependence in SERS using DNA strands elucidates the characteristics of the localised plasmons. Changes in electrochemical potential add another dimension to the understanding at the molecular level and highlight the advantage of these engineered plasmonic SERS substrates [2].

Using the same substrates as the template we further show that using elastomeric polymers, flexible plasmonic structures can be created using nanoimprinting, which allow dynamic and reversible tuning of plasmonic resonances. This is possible due to the size and geometry dependence of localised plasmon resonances in nanostructured cavities [3]. The same idea is extended to arrays of nanoparticles, where plasmon resonances depend both on particle size and inter-particle spacing, and are also shown to exhibit mechanically tuneable resonances [4]. This mechan-optical tunability opens up new applications for engineered plasmonic structures.

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On the Optical Conductance of Tapered Fibers

INCLAN-SANCHEZ Luis[1], MARIANO-JUSTE Marina[2], DOMINGUEZ Jorge L.[2], MARTORELL Jordi[2], SAENZ Juan José[1]

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[2]ICFO-The Institute of Photonic Sciences, Castelldefels, Spain

Understanding the transmission, guiding and loss of electromagnetic radiation in confined optical systems is a key issue in nanoscience and technology. The telecommunication applications need new methods to specify the characteristics of the systems. For example the communication links require a precise calibration of the circular waveguide that has found extensive use in this kind of systems.

The purpose of this work is to discuss wave transport through tapered optical systems using the optical conductance concept. To illustrate the optical conductance concept application to tapered fiber, we present numerical calculations of the waveguiding characteristics for different fibers. Examples of the transmission and dispersion diagram computation with various outer cladding refractive indexes and tapered profiles are investigated in this work.

The property of interest to the present application involves the possibility that the tapered fibers could be used to obtain useful information about the geometry of the systems by means of optical conductance measurements. Preliminary experimental results for some tapered fiber examples will be presented at the conference.

29 SEPT. | 15:00 | Poster Session

Near field local enhancement by ordered arrays of sub-wavelength scattering centres fabricated by femtosecond ablation

LAMELA J.[1], BARRIO J.[1], RODENAS A.[1], ZHOU G.[2], LIFANTE G.[1], JAQUE F.[1], JAQUE D.[1], GU M.[3]

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Controllable light focusing at the nanoscale is one of the most difficult challenges that modern nano-photonics is nowadays facing since it is required for a large variety of practical applications including sub-wavelength imaging, high density data storage, signal processing, non-contact nanosensing, nanolithography and single molecule applications. Light enhancement at the nano-scale is not an easy task since it implies beating the fundamental Abbe´s diffraction limit. Plasmon-supporting metallic nanostructures and ordered arrays of metallic diffraction elements have been already successfully used for this purpose.

Nevertheless, Near Field Enhancement (NFE) is not only interesting in metallic based systems but also in optically active transparent crystals since it would constitute the first step towards the development of novel devices such as low threshold nano-lasers, luminescent nano-modulators, nanosensors, and selectively pumped photonic crystals. Despite of its interest, NFE in transparent crystalline devices is still an open question. Due to the absence of metals, NFE should invoke new fundamental processes different from plasmon wave interferences. Although several approaches (such as the use of surface self assembled nanoscale spherical lenses arrays) have been already proposed, the use of new direct fabrication technologies becomes necessary in order to induce NFE into device substrates.

In this work we show how the ultrafast laser inscription of nanohole arrays enables near field local enhancement in high refractive-index crystals. We first demonstrate both experimental and theoretically how when two nanoholes are separated by intermediate distances (700-1000 nm), near field interference can take place resulting in a near-field enhancement between nanoholes. Based on this effect, near-field enhancements close to a 60% are then demonstrated at the centre of nanohole arrays, and strong optical contrasts in excess of 100% are produced. The integration of these arrays into crystal substrates provides a versatile tool for new optical trapping and evanescent-field nanosensing devices.

Acousto-plasmonic dynamics of metallic nano-objects

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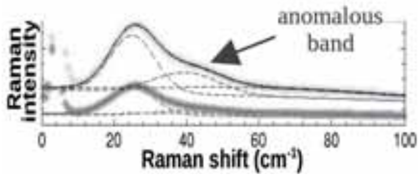
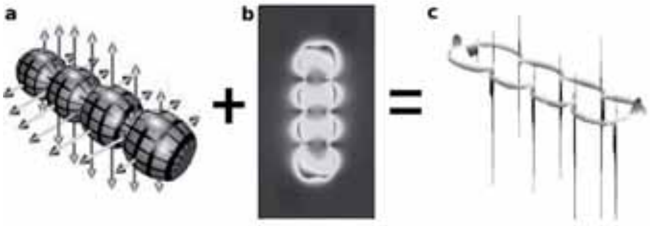
We experimentally observe an unexpectedly strong acoustic vibration band in the Raman scattering of silver nanocolumns (NCls), usually not found in isolated nano-objects. The frequency and the polarization of this unexpected Raman band allow us to assign it to breathing-like acoustic vibration modes. To understand this "anomalous" Raman scattering, we address a theoretical and experimental study of the interactions between acoustic vibrations and localized surface plasmons (LSP). The modulation of the LSP nearfield allows for the interpretation of experimental Raman-Brillouin spectra in these NCls.



Based on full electromagnetic near-field calculations coupled to the elasticity theory, we introduce a new concept of "acousto-plasmonic hot spots" which arise here because of the indented shape of the NCls. These hot spots combine both highly LSP and strong shape deformation by the acoustic vibrations at specific sites of the nano-objects. In order to investigate this new concept, we integrate the Boundary Element Method for the electromagnetic calculations and the elasticity theory by the means of the RUS method for the vibrational calculations which allows calculating the modulation of the LSP polarization for these acoustic vibrations.



We show that the interaction between breathing-like acoustic vibrations and surface plasmons at the "acousto-plasmonic hot spots" is strongly enhanced, turning almost silent vibration modes into efficient Raman scatterers. The indentations of the silver NCls are responsible for the strong localization of the LSP nearfield and its modulation by breathing-like acoustic vibrations. The concepts, the numerical and experimental approaches developed here are not specific to indented NCls and can be extended to other isolated nano-objects exhibiting strong field localization, dimers and more complex metallic nanostructures combining size, shape and interaction effects.

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Fano Resonances in Plasmonic Nanoclusters: Geometrical and Chemical Tunability

LASSITER J. Britt[1], SOBHANI Heidar[1], FAN Jonathan A.[2], KUNDU Janardan[1], CAPASSO Federico[2], NORDLANDER Peter[1], HALAS Naomi J.[1]

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Clusters of plasmonic nanoparticles and nanostructures support Fano resonances. This spectral feature, produced by the interference between bright and dark modes of the nanoparticle cluster, is strongly dependent upon both geometry and local dielectric environment. This permits a highly sensitive tunability of the Fano dip in both wavelength and amplitude by varying cluster dimensions, geometry, and relative size of the individual nanocluster components. Plasmonic nanoclusters show an unprecedented sensitivity to dielectric environment. In this poster we will show that heptamers, planar nanoclusters consisting of seven individual nanoparticles, can display a local surface plasmon resonance (LSPR) figure of merit of 5.7, the highest yet reported for LSPR sensing in a finite nanostructure. We will then explore the possibility of using nanoclusters that are asymmetric or consist of eight or more nanoparticles to achieve even higher sensitivities and new approaches for dielectric sensing.

Poster Session | 15:00 | 29 SEPT.

Magnetic modulation of the real and imaginary part of SPP wavevector in Au/Co/Au films

MARTIN-BECERRA Diana[1], GONZALEZ-DIAZ Juan B.[1], TEMNOV Vasily V.[2], CEBOLLADA Alfonso[1], ARMELLES Gaspar[1], THOMAY Tim[3], LEITENSTORFER Alfred[3], BRATSCHITSCH Rudolf[3], GARCIA-MARTIN Antonio[1], GONZALEZ María U.[1]

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Surface plasmon polaritons (SPP) constitute a promising route towards the development of miniaturized optical devices. To satisfy all the needs in the implementation of nanophotonic circuits, both passive and active elements are required. An active plasmonic system demands a controlling agent able to modify the SPP properties. It has been recently demonstrated that it is possible to obtain active plasmonic modulators with the magnetic field as the control agent based on plasmonic interferometers engraved on Au/Co/Au multilayers [1]. The interferometers consist of a tilted slit-groove pair. When illuminating them with *p*-polarized laser light, the spatial distribution of transmitted light intensity shows a periodic optical interference pattern along the slit axes due to excitation of SPPs propagating between the slit and the groove. By applying an external oscillating magnetic field the magnetization in the cobalt layer is periodically switched thus changing the SPP wavevector and shifting plasmonic interference fringes, which results in an intensity modulation (magnetoplasmonic signal). In that previous work [1], it was analyzed the modulation of the real part of the SPP wavevector for different Co positions and for a single wavelength. But actually, the effect of the magnetic field in those systems is the modulation of both the real and the imaginary part of the SPP wavevector. The modulation of the real part is related to the amplitude of the magnetoplasmonic intensity, while the modulation of the imaginary part induces a phase shift between the optical and the magnetoplasmonic signals.

Here we will present a detailed analysis of the evolution of these two modulations with the Co layer position for different wavelengths. We have observed that the modulation of the real part decreases as wavelength increases, while that of the imaginary part shows a more complex behavior.

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29 SEPT. | 15:00 | Poster Session

Symmetry forbidden infrared resonances in single metallic nanoantennas

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Individual gold nanoantennas prepared by electron beam lithography were investigated by means of microscopic infrared spectroscopy. Contrary to our expectations, we observed not only the well known fundamental antenna-like mode, but also even higher order resonances in the infrared relative transmittance spectra taken under normal incidence of light. The excitation of even modes should not be possible with infrared radiation under the given experimental conditions since modes of even order are dipole-forbidden due to their centro-symmetric charge density oscillation. Performing atomic force microscopy we clearly attributed the appearance of such dipole-forbidden modes to structural deviations of the nanoantennas from an ideal shape that break the symmetry. Further, we performed calculations using the boundary element method, which are in good agreement with our experimental results on the defect induced activation of dipole-forbidden modes.

Poster Session | 15:00 | 29 SEPT.

Optical spectroscopy of conductive molecular junctions in plasmonic cavities

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In the last decade fundamental advances have been achieved in the fields of molecular electronics[1] and plasmonics[2]. Recent simultaneous measurements of electronic conduction and Raman spectroscopy in molecular junctions have suggested the possibility of sensing individual molecules[3], connecting both fields.

We study theoretically this connection in a system composed of a conductive molecular junction bridging a plasmonic cavity formed by two gold nanoshells. These nanoparticles are formed by a silica core surrounded by a gold shell and the molecular junction is modelled as a cylinder linking both nanoshells. The conductivity of the junction is related to its conductance through geometrical parameters. Therefore, for a given size of the linker, we modify its conductivity varying the number n of quanta of conductance, nG_0(G_0º$2e^2/h$@77.5mS). Optical extinction spectra are obtained solving Maxwell's equations via a Boundary Element Method (BEM)[4].

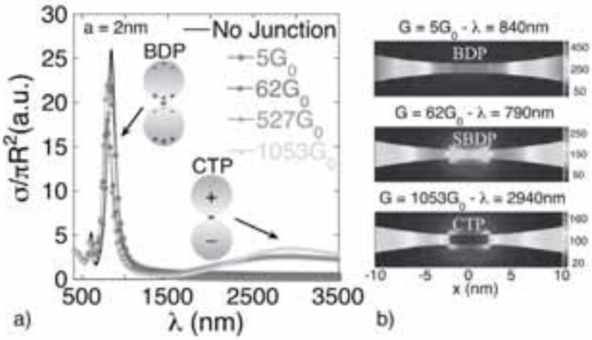

Figure: (Left) - Optical extinction spectra of a nanoshell dimer bridged by a conductive molecular junction of radius a = 2nm as conductivity is increased via the increment of conductance. (Rigth) - Near-fields patterns corresponding to the short wavelength regime (up and medium) and to the long wavelength regime (down), where the progressive expelling of the electric field out of the junction can be observed.

We find two regimes in the optical response (Figure), the Bonding Dimer Plasmon (BDP) for short wavelength values and the Charge Transfer Plasmon (CTP) for longer wavelength values. As conductance is increased, we first notice a broadening of the BDP, followed by a slight blue-shift until a saturation point is reached. Then, the resonance becomes narrower again as conductance continues its increment while its wavelength remains unaltered. For long wavelength values, there is no appreciable change until very large values of conductance are considered, when the CTP, highly red-shifted, emerges.

We believe that this study of spectral changes in plasmonic cavities might serve as a probe of molecular conductance and transport processes in the visible spectrum, a range not accessible through electrical measurements.

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INFRARED PHONONIC NANOANTENNAS: Surface Phonon Polaritons in SiC Disks.

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Infrared light interacts with interfaces of phononic materials through the excitation of surface phonon polaritons. The interaction of infrared light with nano/micron sized particles of polar materials forming localized surface phonon polaritons cause antenna effects, like enhanced absorption and scattering of electromagnetic radiation in some particular frequencies and enhancement & localization of electromagnetic field, allowing micron sized-structures of polar materials to act as nanoantennas in the infrared. We study the optical response of micron-sized SiC disks as nanoantennas in the infrared, using the Boundary Element Method to solve exactly Maxwell's Equations. The size and thickness dependence of the electromagnetic resonance of SiC disks with radius ranging from 400 nm to 600 nm and thickness ranging from 50 nm to 100 nm is studied. The interaction of a metallic probing tip with the nanoantenna, which is of interest in nanoscale microscopy, is also studied. The calculations also give hints on superlensing effect shown by polar materials in the infrared.

Designing metal nanoantennas though bio-inspired stochastic optimization

RODRIGUEZ-OLIVEROS Rogelio[1], SANCHEZ-GIL Jose Antonio[1], TASSADIT Abdelwahab[2], MACÍAS Demetrio[2], ADAM Pierre Michel[2]

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[2]Laboratoire de Nanotechnologie et d´Instrumentation Optique (UTT) Institut Charles Delaunay, Troyes, France

In this work a method is developed to design nanostructures at will, based on a bio-inspired stochastic algorithm to optimize configurations for a given electromagnetic property. In particular, we proof the suitability of the method by finding the optimal geometry that maximizes, for a fixed wavelength, the scattering cross section of a bi-dimensional metal nanostar. The "genetic" operations of recombination and mutation are applied over the elements (parameters to be optimized) of the initial population. Recombination exploits the search space through the exchange of information between different elements population. Mutation, on the other hand, explores the search space through the introduction of random variations in the newly recombined elements. To solve the scattering problem for each particular realization of the parameters, we employ a rigorous numerical method based on Green´s theorem surface integral equations, where the nanostar shape is generated through Gielis' formula. It is shown that the optimization procedure with specific evolution strategy converges satisfactorily to a nanostar geometry that exhibits a resonance at or near the given wavelength. The influence of the illumination conditions, the effect of geometries found on the near-field features are also explored. Furthermore, the potential application of our approach to Nanophotonics design will be discussed for a variety of configurations.

| 29 SEPT. | 15:00 | Poster Session |

Absorption enhancement in light-harvesting complexes coupled to plasmons in a silver island film: experiment and theory

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Nanotechnology provides nowadays many ways to externally tune the optical properties of biomolecules, including light-harvesting complexes [1]. In this work we study theoretically and experimentally the influence of plasmon excitations upon peridinin-chlorophyll-protein (PCP), a light-harvesting complex from Amphidinium carterae [2].

The PCP complexes were deposited on a Si02 25-nm thick spacer, which separated the complexes from a silver island film (SIF). The plasmon resonance of the SIF was about 450 nm. The results of fluorescence spectroscopy show large enhancement of the absorption of the complex, while exciting the plasmons in the SIF.

In order to interpret the data, we generalize a traditional scheme [3-4] of the molecule-metal interaction to the case of a PCP-molecule with two interacting dipoles placed in the vicinity of a metal nanoparticle. The calculated optical responses involve both intra-PCP energy-transfer dynamics and the dipole-metal interaction.

SIF constitute a distribution of sizes and shapes of MNPs. By tuning the incident light wavelength to the plasmon resonance of chosen group of particles, we create a rapidly-varying scattered electric field distribution over the SIF surface. In the theoretical analysis we focus on light absorption efficiency of light-harvesting complexes placed over SIF. The results of modeling quantitatively agree with the experimental data. Modeling includes several elementary processes, such as FRET in the PCP molecule, absorption enhancement, fluorescence quenching due to non-radiative energy transfer to metallic nanoparticles (plasmon-induced FRET), and light scattering on MNPs.

This work is supported within the research project WELCOME "Hybrid nanostructures as a stepping-stone towards efficient artificial photosynthesis" awarded by the Foundation for Polish Science.

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Poster Session | 15:00 | 29 SEPT.

Mapping and Control of Nanoscale Optical Vector Fields

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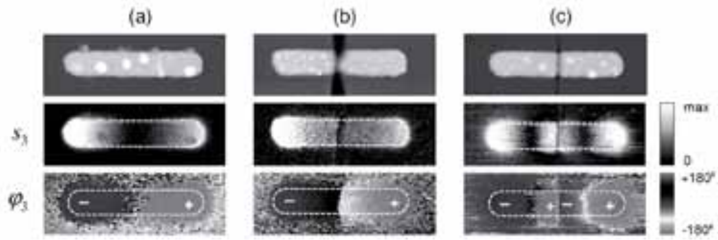
We demonstrate nanoscale resolved mapping of the near-field distribution of optical antennas by scattering-type scanning near-field optical microscopy (s-SNOM). Polarization-resolved interferometric detection yields amplitude, phase as well as the direction of the local electric fields, allowing for the complete characterization of the polarization state of nanoscale confined light fields such as found in antenna gaps. Particularly, the use of sharp Si tips with tip radius < 20nm allows for accessing the near fields *inside* nanoscale antenna gaps < 100 nm, which is essential for identifying regions of high field concentration (hot spots) generated by the antenna.

We apply vector near-field mapping to study how the optical response of IR nanoantennas can be controlled by targeted manipulation of the antenna gap (see Fig). To this end, we prepare a series of metallic nanorods with a central, isolating gap and successively load the gap with metal bridges of varying diameter. By mapping the antenna near fields, we provide direct experimental evidence that the diameter of the gold bridges controls the optical response of the entire nanoantennas. We show that circuit theory concepts can be adapted from the radio frequencies to the infrared regime in order to describe the control of gap loading on the antenna response. It is the combination of targeted antenna loading and circuit theory that can provide a new tool for a versatile design of antenna near-field patterns, which could be highly valuable for the development of compact and integrated nanophotonic devices.



29 SEPT. | 15:00 | Poster Session

Coloring fluorescence emission with silver nanowires

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We demonstrate that emission from Rhodamine-6G fluorophores adsorbed on silver nanowires experiences a spectral redshift upon propagation to the distal ends of the nanowire, with the shift being proportional to the propagation distance. The end of a nanowire thus constitutes a tunable fluorescence source controlled by a single easily adjustable parameter, i.e., the position of the excitation focal spot. The effect is made possible by a combination of radiatively undamped plasmon propagation and dispersive ohmic losses in the silver nanowire. The results may be important for the development of plasmonic waveguides, fast fluorescent color switches and various nanoscale fluorescence sensors.

Spontaneous Emission Control of Semiconducting Nanocrystals and Dye-Molecules Embedded in Nanoimprinted Polymer Photonic Crystals via Localized Surface Plasmons

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We report on a universal method to enhance the light-emission efficiency of printable thin films of polymer doped with emitters by coupling their exciton to localized surface plasmon generated by metallic nanoparticles embedded in polymer matrixes. In this work we use small amount of Au nanorods with a double surface plasmon resonance in a solution of R6G and of CdSe(ZnS) nanocrystals We demonstrate that our approach can dramatically enhance the photoluminescence of dye chromophores and of semiconducting nanocrystals, here shown probably for the first time in a blended polymer, by carefully controlling the distance between emitters and metallic nanoparticles. A reduction of the lifetime confirmed the modification of the spontaneous emission rate of the emitters. A higher photoluminescence enhancement can be achieved by patterning the nanocomposite polymer with photonic crystal (36-fold). A numerical model has been developed to understand the complex exciton/plasmon coupling phenomena. The method is based on the Green´s function formalism to calculate the optical field and molecular decay rate, and on the optical Bloch equations formalism for the evolution of the internal state of the molecule. Our investigation allows to separate different contributing factors such as the modification of radiative decay rate, the local fields modification, the absorption variation and the far-field extraction enhancement.

29 SEPT. | 15:00 | Poster Session

Nanoscale Free-Carrier Profiling of Individual Semiconductor Nanowires by Infrared Near-Field Plasmon Resonance Spectroscopy

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We report nanoscale mapping of free carriers in single semiconductor nanowires by infrared (IR) near-field Plasmon-Polariton resonance spectroscopy. Local Plasmon-Polariton spectroscopy is performed by scattering-type Scanning Near-field Optical Microscopy (s-SNOM).

Our s-SNOM [1] is based on Atomic Force Microscopy (AFM) where the tip is illuminated with a focused laser beam and the tip-scattered light is detected simultaneously to topography. Combining higher harmonic demodulation with interferometric detection allows for background-free near-field imaging in amplitude and phase. Using metalized tips, the strong optical near-field concentration at the tip apex can excite local oscillations of the free carriers (Plasmon Polaritons) at the sample surface, yielding a characteristic spectral signature of the tip-scattered light. The spectral position of this near-field induced plasmon resonance occurs close to the plasma frequency of the free carriers and shifts to higher frequencies with an increasing free-carrier concentration n. Using s-SNOM we study the free-carrier properties in single modulation-doped InP nanowires, which were grown using the vapor-liquid-solid (VLS) method. By fitting these spectra with model calculations using n as a fitting parameter, we can determine the local free-carrier concentration n. Imaging nanowires as thin as 20 nm, we find local variations of the free-carrier concentration, which can be attributed to local growth defects [2].

With s-SNOM we provide a contactless, non-destructive optical nanoscopy tool, which allows quantitative measurement of the free-carrier concentration in semiconductor nanowires with nanoscale spatial resolution. Improved modeling and spectral extension of s-SNOM to the THz frequency range [3] could make the method a powerful tool for free-carrier profiling not only of nanowires, but also of other semiconductor nanodevices and photonic nanostructures.

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Poster Session | 15:00 | 29 SEPT.

Photonic Hall-effect for a single nanoparticle

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Quantum Hall effect arises when electrons are subject to a large magnetic field due to the fact that electrons experience a Lorentz force as they are charged. Despite the absence of photonic charge, it has been observed that a similar effect, a photonic Hall-effect, appears when light is subject as well to a magnetic field, although the origin of the effect is very different.

This photonic Hall-effect, or magneto-transverse anisotropy, in light scattering, is of actual interest and is the basis of interesting phenomena [1,2]. The Hall effect of a single scatter is important by itself. In particular, Hall effect for a Mie sphere has been addressed long before [3]. In these studies it was argued that in the small particle regime (the so called Rayleigh scattering regime) there were no net magneto-transverse scattering effects [3].

Radiative corrections have shown to be important to analyze magneto-optic properties of small nanoparticles [4]. As we will show, Optical Hall-effect in small dipolar particles does exist, arising as a consequence of the radiative corrections to the polarizability.

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29 SEPT. | 15:00 | Poster Session

Incorporation of Inorganic Nanorods into Cholesteric Liquid Crystals for Lasing Application

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Typically a liquid crystal (LC) laser consists of a liquid crystalline host and an organic fluorescent laser dye where the LC provides the feedback and the laser dye provides the gain. Because of the refractive index modulation along the helical axis in cholesteric LC, light cannot propagate within the photonic band gap (PBG), but is rapidly enhanced at the band edges when emitted from inside, due to the photon group velocity tending to zero and the photon dwell time is significantly increased.

In our point of view the usage of an organic laser dye is a disadvantage because of bleaching with time in these systems which need to be pumped with laser light of high intensities. We work on the replacement of the organic laser dye by fluorescent CdSe@CdS nanorods which are chemically inert and very stable towards light, soluble in organic solvents and provide a very high quantum yield.

To incorporate these nanorods the liquid crystalline host needs to be modified in certain ways. First of all, only polymeric mesogens are able to orient nanorods of 50 - 100 nm in length. In a mixture with a solvent the lyotropic LC exhibit a cholesteric phase and no orientation layer is needed as is usual for low molar mass mesogens, because of the huge aspect ratio of these mesogens. On the contrary for a uniform planar alignment the glass subtrates need to be covered with an alignment layer. If the solvent is polymerizable and an UV-initiator is added, the cholesteric phase can be "locked in" after tuning its properties via temperature, mechanical stress, concentration or mesogen length by UV-polymerization.

These composite films with "frozen" cholesteric structure are then insensitve for external stimuli and can be analized without changing pitch because of heating while they are optically pumped.

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