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Spanish Molecular Electronics Symposium

March 24, 2006

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Nanoelectronics represent a strategic technology considering the wide range of possible applications. These include telecommunications, automotive, multimedia, consumer goods and medical systems.

Many of the potential molecular electronic applications still require substantial work in order to be transformed into marketable technology. A concerted effort must therefore be made at the European level to both understand and commercialise atomic scale technology in order to maintain a competitive advantage for Europe and keep Europe at the forefront of the next nanoelectronics revolution, a revolution beyond nanotechnology.

In order for the field of molecular electronic to continue growing exponentially worldwide and therefore lead to new commercial applications and to change the micro and nanoelectronics paradigm, it is necessary to educate new researchers who can work across traditional disciplines. High-level dissemination activities such as SMS 2006 will help to establish a critical mass of R&D at a European level and to stimulate development of an interdisciplinary community of researchers.

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Schottky in Gold- and Palladium-contacted semiconducting carbon nanotubes

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Magnetic and conducting molecular materials

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Supramolecular self-assembly of linear polyarene molecules with complementary imide and amide end groups

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Force Microscopy Investigations Of Molecules

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Combining ab-initio and semi-empirical approaches for STM simulation of molecules weakly bonded to surfaces

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Resistive and rectifying effects of pulling gold atoms at thiol-gold nano-contacts

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Contacting single molecules with the STM: model systems for molecular electronics

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Break junctions in liquid for molecular electronics

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Advancing in the structuring and patterning of single-molecule magnets on surfaces

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Organic Molecules On Surfaces Studied By STM: Dynamics, Chirality And Organization

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NANO2006 Workshop

PERSPECTIVES IN NANOSCIENCE AND NANOTECHNOLOGY

September 4-6, 2006

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The aim of this multidisciplinary workshop is to assess the state of the art in the current understanding of nanoscale physics, chemistry, engineering, biology, and medicine, and to access the knowledge and advice from leader scientists in these fields. We also intend to discuss emerging applications with potentially significant impact for the materials, electronic, photonics, and life-science industries, and to debate about the current strategy and perspectives in Nanoscience and Nanotechnology.

The programme of the workshop is built up around a number of invited talks and contributed papers (oral and poster), with ample time for discussion. The topics of the sessions will include various aspects of nanoscale physics, chemistry, engineering, biology, and medicine, with special emphasis on the synthesis, assembling and manufacturing of nanostructured materials, the development of nanodevices and its impact on molecular electronics, spintronics, nanomagnetism and nanophotonics, and the use of biofunctional nanoparticles in nanobiotechnology and medicine.

The workshop is sponsored by the Donostia International Physics Center (DIPC) and the “Consejo Superior de Investigaciones Científicas” (CSIC), and also by the Basque Government in an effort to launch an initiative to build a new Center of Nanoscience and Nanotechnology (CIC nanoGUNE Consolider). This event takes place in the framework of the Summer Courses of the University of the Basque Country. We are also grateful to the members of the Scientific Committee.

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Photonic metamaterials: Optics starts walking on two feet

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Nanophotonic devices and techniques for sensing applications

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Plasmonic nanostructures from artificial molecules to active nanodevices

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Photonic metamaterials: Nano-scale plasmonics and super lens

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Plasmonic substrates for surface enhanced spectroscopies

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Directed sub-wavelength imaging in a layered metal-dielectric system

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Small is different: from nano-lubrication and jets to correlated electrons in quantum dots

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Mechanics at single atoms & nanoimprint for lithography

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Device integration of semiconductor and magnetic nanostructures

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The research agenda of the EU NoE PHOREMOST: Nanophotonics to reach molecular-scale technologies

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Multifunctional carbon nanotube composite fibers

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Nanowires and suspended atomic chains from Au-Ag alloys

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Perspectives of controllable nanoparticles in diagnosis and therapy

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Biofunctionalized surfaces to study membrane bionanomachines

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Near-field scanning fluorescence microscopy: a nano-tool to investigate the nanoscale organisation of the cell membrane

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Voltage regulation of single molecule fluorescence

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When Things Get Small**Electronic structure** Chair: Prof. Andrés Arnau (UPV/EHU, Spain)

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Advances towards surface-state nanoelectronics

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Structure and electronic properties of hydrogen clusters, free and deposited on graphitic surfaces

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Self-organized nanomagnets and organic molecules at surfaces

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One-dimensional quantum wells in noble metal surfaces and nanostructures

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Electronic and optical properties of self-assembled quantum dots in nanomechanical oscillators**Nanoelectronics** Chair: Prof. Gonçal Badenes (ICFO-The Institute of Photonic Sciences, Spain)

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CMOS trends for the Nanotechnology era

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Electron transport in silicon based nano-transistors

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Electronic and scattering properties of dopants in silicon nanowires

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Nanoscience: Geometry in the laboratory**Nanomagnetism** Chair: Dr. Fernando Plazaola (UPV/EHU, Spain)

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Orbital magnetism in Au and ZnO nanoparticles

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Magnetic logic devices for ultra high density data storage

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Multilayered magnetic ring devices for memory and logic applications**PARTICIPANTS**

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Confinement: Universal Aspects in Soft Matter

December 12-13, 2006

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The effect of “confinement” —i.e. geometrical restrictions— on the dynamics of fluids and glass-forming liquids has received much attention over last decade. Dynamics in confinement appears in a wide range of science: chemistry, physics, materials science, biology, etc. However, most of the recent activity was devoted to glass-forming systems and the question of the possible characteristic length scale for the glass-transition. A new strong move in this field came from the recent general interest in nano-science and nano-technology. The nanometer scale - i.e., the molecular scale - emerges as the most interesting range also for the confined geometries. On the other hand, confinement effects are becoming important in systems where the confined geometries are ill defined (water-biopolymers, multicomponent polymer materials, soft matter systems, etc). The idea of this SoftComp workshop is just to explore the “universal” aspects (if any) of confinement effects in fluids and soft matter. In this brief introduction to the workshop I will try to present some naïve reflections from a non-expert in the field.

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Why Confinement?

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Effect of nanoscopic confinement on the dynamics of glass-forming liquids and polymers.

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Effect of asymmetric Component Mobility on Thermal Composition Fluctuations in the PEO/PMMA Blend.

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Dynamic confinement effects in a blend of poly(ethylene oxide) with poly(vinyl acetate).

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Colloidal Dynamics close to Walls.

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Slow dynamics in confinement: A mode-coupling theory.

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Confinement in simple binary systems with and without connectivity.

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Effective colloidal interactions at fluid interfaces.

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Effect of confinement on droplet dynamics in two-phase polymer blends.

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SoftComp Area 4 Meeting

December 14, 2006

ORGANIZER

Prof. Juan Colmenero (Universidad del País Vasco/Euskal Herriko Unibertsitatea, Donostia International Physics Center, Centro de Física de Materiales-CSIC, Spain)

SoftComp (Soft Matter Nano-Composites) is part of the European Network of Excellence (NoE) which aims to establish a knowledge base for intelligent design of functional and nanoscale soft matter composites. SoftComp is organized for various areas covering different but related aspects of soft materials. In particular, the Area 4 Meeting deals with complex materials based on polymers. Each SoftComp Area meets twice a year to discuss the progress made on the different projects and to plan future activities accordingly. The December 2006 meeting of Area 4 took place in San Sebastian at the DIPC, organized by Professor Colmenero, coordinator of this Area.

CONTRIBUTIONS

J. Oberdise (LCVN, Université Montpellier 2, France)

New reverse Monte Carlo modelling of interacting aggregate structure in nanocomposites.

A. Alegria (Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain)

New dielectric results on PI-branched polymers: Dendrimers vs. other architectures.

G. Schwartz (Donostia International Physics Center, Spain)

An Adam-Gibbs based model to describe the single component dynamics in miscible polymer blends under hydrostatic pressure.

D. Richter (IFF-FZ, Forschungszentrum Jülich, Germany)

Future perspectives.

W. Paul (Johannes Gutenberg-Universität Mainz, Germany)

The point of view from the simulation & theory platform.

W. Pyckhout-Hintzen (IFF-FZ, Forschungszentrum Jülich, Germany)

Perspectives of time-resolved small angle neutron scattering.

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20th Symposium on Surface Science 3S07

March 11-17, 2007

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G. Thornton (London, United Kingdom)

E. Tosatti (Trieste, Italy)

I. Tsong (Tempe, Arizona, USA)

P. Varga (Vienna, Austria)

Since the foundation of this meeting in 1983 as a winter school by the Institut für Allgemeine Physik of the Technical University of Vienna, the format of the meeting has been chosen similar to the Gordon Conferences with ample time for discussion, outdoor activities, as well as attendance below 100 participants. Its aim is to facilitate the exchange of ideas among scientist in the field of surface science and related areas.

CONTRIBUTIONS

Molecules at Surfaces I Chair: P. Ruffieux

J.I. Pascual

Growth of donor-acceptor complexes on metal surfaces

W.A. Hofer

Fun with dipoles: structuring, changing, and switching
Semiconductor surfaces with polar molecules

C. Ambrosch-Draxl

Surfaces and interfaces of organic semiconductors: the importance of van der Waals interaction

Electrons at Surfaces I Chair: B. Hellsing

P. Hofmann

Quantitative measurements of surface conductance using microscopic four point probes

P. Ordejón

Analysis of scanning tunnelling microscopy images of the chargedensity-wave phase in
quasi-one-dimensional Rb_{0.3}MoO₃

Self-Assembly I Chair: G. Thornton

A. Götzhäuser

High thermal stability of cross-linked aromatic self-assembled monolayers:
Nanopatterning via selective thermal desorption

M. Berglin

Structure information in thin organic films by combining quartz crystal microbalance with
dissipation monitoring (QCM-D) with surface plasmon resonance (SPR)

M. Buck

Electrochemical nanotechnology: Studies on metal deposition controlled by self-assembled
monolayers

Self-Assembly II Chair: T. Greber

R. Fasel

Molecular self-assembly on nanostructured template surfaces

K.J. Franke

Tuning the interaction of fullerenes with metal surfaces by molecular self-assembly

N. Lorente

Properties of fullerene-base molecular structures on metal surfaces

Ion-Surface I Chair: F. Aumayr

M. Descoins

Ion projection microscopy using a coaxial structure point source

J.R. Manson

Atomic and Molecular Collisions with Surfaces: Comparisons between Ar and N₂ Scattering from
Ru(0001)

Friction Chair: U. Heinzmann

H. Brune

Nanotribology-between kinetics of Capillary Condensation and Atomic Stick and Slip Motion

S. Yu. Krylov

Delocalization of nano scale mechanical contact: Do we get what we see in atomic friction?

Electron States at Surfaces II

Chair: P. Ordejón

H.-C. Ploigt
Scanning tunnelling spectroscopy of image potential states on NaCl/Ag(100)

C. Ast
Local detection of spin-orbit splitting by scanning tunnelling spectroscopy

P. Brodard
Morphology and Electronic Structure of Self-Assembled Azure A Molecules on Au(111) investigated by Low-Temperature UHVSTM

Poster Presentations

Chair: W.-D. Schneider

N. Gonzalez Lakunza Self-Assembly of heterogeneous supramolecular structures with uniaxial anisotropy

L. Gorelik Charge solitons in monolayer of colloidal quantum dots onto metal surface

T. Greber Hydrogen in C60

A. Leonardo Quantum well states as Fabry-Pérot modes in Mg/W(110)

U. Narkiewicz Elimination of carbon from TiC/C nanocomposites through hydrogen treatment

P. Ruffieux Site-specific adsorption of polycyclic aromatic hydrocarbons

A. Saúl Monoatomic metallic wires: structure, electric transport and normal modes

V. M. Silkin The role of surface state in the surface response function of metals

G. Teobaldi Lepidocrocite titanium oxide ultrathin film on Ni(110) first principle modelling and simulated STM imaging

D. Sanchez-Portal First-principles calculations of nanostructured surfaces: metal-insulator transition in the Si(557)-Au surface

L. Lapena Coupling between structural and chemical phase transition during Sb/Si(111) adsorption

P. Müller Spirals on Si(111) at sublimation and growth: first experimental evidence of deviations to the usual BCF behaviour

Electron-Phonon Coupling

Chair: P. Hofmann

B. Hellsing
Electron-phonon coupling and its influence on electron and phonon lifetime at surfaces

E. V. Chulkov
Phonon spectra and electron-phonon coupling in a monolayer structure of Na on Cu(111)

Adsorbate Interactions at Surfaces

Chair: K. Morgenstern

N. V. Richardson
How circular is coronene? Weak 2D anisotropy leading to chirality in highly symmetric systems

G. Thornton
Molecular side hopping on an oxide surface

L. Diekhöner
Magnetic exchange coupling between single atoms

Surface Structure II

Chair: N.V. Richardson

P. Varga
Structure of the $\sqrt{67} \times \sqrt{67}$ (surface oxide on Ni) R12.2O 3Al(111)

F. Mittendorfer
Oxygen induced surface roughening of Rh(322)

J. Hrbek
STM and XPS study of growth of Ce and CeOx on Au(111)

Semiconductor Surfaces

Chair: W. A. Hofer

I. S.T. Tsong
Optical studies of Si_{1-x}Ge_x Nanodots

F. Leroy
Self-ordering by electromigration

Theoretical Methods

Chair: N. Lorente

M. Scheffler
Key Theoretical and Algorithmic Needs for Predictive Modelling of Surface Chemistry and Catalysis

K. Reuter
On the accuracy of first-principles lateral interactions: Oxygen at Pd(100)

Molecules at Surfaces II Chair: H. Brune

P. Cabrera-Sanfelix

Two dimensional Chlorine solvation on NaCl(100) at low Relative Humidity

A. Mugarza

Understanding the adsorption of water molecules on Ru(0001) and their interaction with co-adsorbed oxygen by low temperature scanning tunnelling microscopy

K. Morgenstern

Determination of non-adiabatic barriers for diffusion and attraction of molecules with a fs-STM

Miscellaneous I Chair: N. Müller

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Attosecond time-resolved photoemission on metal surfaces

Andy T. Wu

Surface Study of Niobium for Superconducting Radio Frequency Cavities at Jefferson Lab

K. Miki

Bi nanoline on Si(001) surface and its application to onedimensional epitaxial growth or cluster formation as a template

Surface Structure II Chair: P. Varga

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Real space direct visualization of the layer-dependent roughening transition in nanometer-thick Pb films

J. A. Smerdon

Formation of a quasicrystalline Pb monolayer on a range of quasicrystal surfaces

Miscellaneous II Chair: I.S.T. Tsong

A. Biedunkiewicz

Nanocrystalline TiN coatings on Al₂O₃

H. van Beijeren

Finite size effects on equilibrium shapes due to line tensions

Ion Surface II Chair: J.R. Manson

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Nano-hillock formation by impact of slow highly charged ions on various surfaces

D. O. Boerma

Stratified Monte Carlo simulation of ion trajectories in crystalline solids applied to some problems in ion-solid interactions

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IN16B Meeting

May 10, 2007

The DIPC hosted a meeting of representative people from the Institut Laue-Langevin (ILL, Grenoble, France), the Basque Government and several Spanish enterprises. The objective was to discuss the possibilities of collaboration in the development of a neutron scattering spectrometer at the ILL, the backscattering instrument IN16B. IN16B is one of the main targets in the Millennium Project -the Program initiated by the ILL for updating existing instruments or designing new ones, in order to keep the leadership in Europe regarding neutron scattering facilities and offer competitive alternatives to those available soon with the new third generation neutron sources. IN16B would be an extremely useful instrument for the investigation of dynamical processes in condensed matter, providing a very good energy resolution and high neutron flux. In addition, the potential expertise gained by the Spanish community in this collaboration would be very valuable in a near future, if the European Spallation Source (ESS) Project would be attracted to the Basque Country.

CONTRIBUTIONS

H. Schober (Institut Laue-Langevin, Grenoble, France)
The ILL and the Millennium Project

B. Frick (Institut Laue-Langevin, Grenoble, France)
Backscattering techniques: the IN16B Project

D. Bazzoli (Institut Laue-Langevin, Grenoble, France)
Technical details of IN16B

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Ab-initio Approaches to Electron-phonon Coupling and Superconductivity

May 28-30, 2007

ORGANIZERS

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Dr. Igor I. Mazin (Center for Computational Materials Science, Naval Research Laboratory, Washington, DC, USA)

Prof. Warren E. Pickett (University of California, USA)

Dr. Aritz Leonardo (Universidad del País Vasco/Euskal Herriko Unibertsitatea and Donostia International Physics Center, Spain)

The aim of this workshop is to give an overview of recent ab-initio calculations of electron-phonon coupling in superconducting and nonsuperconducting materials, in bulk as well as at the surface. The workshop will cover, for example, linear response calculations of the e-ph coupling resolved both in energy and momentum, the newly developed superconducting density functional theory, and numerical methods of the Eliashberg theory. Important topics like anharmonicity, nonadiabaticity, and unconventional order parameters will also be discussed, as well as spectroscopic effects of the e-ph coupling, e.g., in photoemission. Although the workshop is mainly theoretical, we anticipate having some experimentalists as well, and hope that this will lead to productive cross-fertilization between the theory and the experiment.

CONTRIBUTIONS

G. Bachelet

Electron-phonon interaction in electron-doped graphite

K.-P. Bohnen

Lattice dynamics and electron-phonon coupling in carbon nanotubes

M. Calandra

Superconductivity in graphite intercalated with alkaline earths

S. Curtarolo

First principle search for new superconducting materials

A. Eiguren

Complex quasiparticle structure induced by electron-phonon interaction

R. Gonnelli

Point-contact Andreev-reflection spectroscopy and e-ph coupling in doped and irradiated MgB₂

E.K.U. Gross

How to predict the critical temperature of superconductors

P. Hofmann

The electron-phonon interaction probed by angle resolved photoemission

A. Liu

Electron-phonon coupling in Li₂B₂

S. Massidda

Impurity effects in superconductivity of MgB₂

F. Mauri

Non-adiabatic vibrations in doped graphene

D.A. Papaconstanoupoulos

Effects of pressure on superconductivity in monoatomic metals

I. Sklyadneva

Ab-initio calculations of electron-phonon coupling at metal surfaces

D. Van der Marel

Electron-phonon interaction and charge carrier mass enhancement in n-doped SrTiO₃

O. Gunnarsson

Many-body effects in electron-phonon coupling

O. Fischer

Electron-phonon interaction in Chevrel-type compounds

A. Goldoni

Band dispersion K₆C₆₀(110) and K₃C₆₀(111) films measured with ARPES

I. Mazin

Charge ordering as alternative to Jahn-Teller distortion

A. Fuertes Amparo

Superconductivity in layered zirconium and hafnium nitride halides

W. Pickett

Strong e-ph coupling in elemental metals under pressure: Observations, questions and progress poster

L. Boeri

Interaction in hexagonal layered compounds: alkali earth intercalated graphites and disilicides

J.S. Kim

Superconductivity in alkaline earth-intercalated graphites: CaC₆ and SrC₆

J. Kunes

KOs₂O₆: Superconducting rattler

M. Ellerby

Experimental aspects of superconductivity in intercalated graphites

B. Hellsing

First principles surface phonons and electron and phonon lifetimes at surfaces

A. Bergara

Increasing crystal local-field effects and superconductivity in simple elements under pressure

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Symposium at the 4th European Conference On Neutron Scattering

June 26, 2007

In June the 4th European Conference on Neutron Scattering was held in Lund (Sweden), gathering more than 700 scientists. One of the Symposia of this great event, 'Modelling and Neutron Scattering. Soft Matter and Biology', was sponsored by the Donostia International Physics Center. The aim of this Symposium was to emphasize the potential of the combination of neutron scattering and modelling to unravel the structural and dynamical properties of systems of increasing complexity. Experts covering different areas of soft matter were invited with the financial support of the DIPC and gave excellent lectures. The Symposium was attended by a very large number of participants and a fruitful discussion atmosphere could be enjoyed.

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 A. Wischnewski (Forschungszentrum Jülich, Jülich)
 M. Tyagi (DIPC, San Sebastián)
 M.A. González (Institut Laue-Langevin, Grenoble)

Elementary Reactive Processes at Surfaces

August 30-September 1, 2007

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Dr. Maite Alducin (Donostia International Physics Center, Spain)
 Dr. Heriberto Fabio Busnengo (Universidad de Rosario, Argentina)
 Dr. Ricardo Diez Muino (Centro de Física de Materiales-CSIC, Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain)

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 Dr. Daniel Farias (Universidad Autónoma de Madrid, Spain)
 Prof. Axel Gross (Universitaet Ulm, Germany)
 Prof. Geert-Jan Kroes (Universiteit Leiden, Netherlands)
 Prof. Mario Rocca (Universita di Genova, Italy)

Stimulated by the success of the Workshop 'Molecule-Surface Interactions: Elementary Reactive Processes', that was held in Donostia-San Sebastian in September 2004, we organized another 3-day Workshop in San Sebastian in 2007. The general subject of the workshop is similar, namely, 'Elementary Reactive Processes at Surfaces'. More specific topics include elementary reactions involved in fundamental and catalytic processes at surfaces, dynamics of atomic and molecular adsorption and desorption, non-adiabatic effects, energy dissipation, self-assembling, surface functionalization, and surface photochemistry. The goal is to bring together researchers actively working in any of these topics and discuss about their recent results, the current status of the field, and future perspectives.

CONTRIBUTIONS

P. Saalfrank

Controlling the photoreactivity of atoms and molecules at surfaces

C. Frischkorn

Ultrafast laser induced dynamics of associative desorption reactions from metal surfaces

T. Klüner

Surface photochemistry from first principles

A. Kummel

Chemical dynamics of gas reactions on organic films in UHV and in ambient air

T. Greber

Formation of single sheet boron nitrides on transition metals

N. Lorente

Dehydrogenation of benzene and pyridine on Cu(100) by tunneling electrons and the inelastic electron spectroscopy identification of the corresponding fragments

R. Beck

Quantum state resolved studies of Silane chemisorption on Si(100)

J.E. Gayone

Direct recoil spectroscopy of alkanethiol covered surfaces

R. Otero

Adsorption, dynamics and self-assembly of organic ad-species for catalytic and photovoltaic applications

E. Martínez Núñez

Inelastic scattering dynamics of Ar and CO₂ on a fluorinated self-assembled monolayer surface

Y. Wang

Understanding the supramolecular self-assembly of the fullerene derivative pcbm on Au(111) surface

S. Iannotta

Kinetic activated processes at surfaces and hybrid structure synthesis by supersonic and cluster beams

L. Vattuone

Adsorption and reaction of aligned molecules at metal surfaces

L.M. Molina

The reaction mechanisms for CO oxidation at gold catalysts: Relevance of realistic reaction conditions

A. Wodtke

Inverse velocity dependence of vibrationally promoted electron emission from a metal surface

E. Pehlke

TDDFT simulations of electronic energy dissipation during chemisorption

C. Carbogno

Spin effects in the adsorption of O₂ on Al(111) surfaces

G. Darling

Surface temperature effects in reactive dynamics

B. Jackson

The role of surface reconstruction in gas-surface reactions

C. Díaz

Multidimensional "high level" calculations for a prototype system: H₂/Cu(111)

G. Bocan

Sticking probability of N₂/W(110) using different exchange correlation functionals

A. Hodgson

H recombination at an ordered SnCu alloy surface: Reaction dynamics in a bistable system

A. Martínez

Dissociative adsorption of H₂ on W and W/Cu: Prominent features of surface alloying

- P. Nieto
Using diffraction to study the Hydrogen dissociation dynamics at metal surfaces
- A. Barinov
Quantum size effect in oxidation of thin Al(111) films grown on W(110) substrate
- H.-J. Freund
Reactions on oxide-supported nanoparticles
- C. Wöll
Elementary reactions at oxide surfaces: Case studies for ZnO
- G. Comelli
STM investigations of elementary reaction steps on the oxydized Rh(110) surface
- L. Guillemot
Nanostructure formation by reaction of H₂O with pre-adsorbed O on a Ag(110) surface
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Efficient Density Functional Calculations: Hands-on Tutorial on the SIESTA Code

November 20-23, 2007

Following the very successful tutorial that took place in CECAM (Lyon) on June 2007, and taken into account that due to restrictions imposed by the European funds used to organize that event many researchers could not attend, we are organizing a hands-on tutorial on the use of the SIESTA program in Donostia-San Sebastian.

This is a four-day hands-on tutorial on the use of the SIESTA code, aimed at researchers from different disciplines who want to use the code in their research and need, apart from basic practice, a grounding on the capabilities of the method and the approximations used. The main goal is that the students understand the physical and main technical approximations behind the method and can assess its reliability and its usefulness for a particular problem. Apart from the basics of density-functional theory, molecular dynamics simulation and geometry relaxation, which are common to most codes, the specific SIESTA topics to be covered are the generation and use of pseudopotentials, the construction of basis sets of strictly localized numerical atomic orbitals, localization issues for linear scaling both in the computation of the matrix elements and in the resolution of the hamiltonian, as well as more technical ones such as the influence of the real-space grid and parallelization. The tutorial will consist of morning lectures followed in the afternoon by a practical "hands-on" session. Some fundamental knowledge of quantum mechanics will be assumed, as well as basic statistical mechanics for the molecular dynamics part. Some solid state physics background will be helpful but not strictly needed. Basic knowledge of UNIX is required.

Talks dealing with the basic theory and methodology behind density functional ab initio calculations and the peculiarities of the SIESTA code will take place in the mornings at Donostia International Physics Center. The hands-on sessions will take place in the afternoons in the computer rooms of the Chemistry building and will try to show how to use the code and its different capabilities with realistic examples.

TUTORIALS

A. García

Introduction: computer simulations, the quantum-mechanical many electron problem and Density Functional Theory

P. Ordejón

Brief introduction to the SIESTA method

E. Anglada

Basic execution (input, output, k-points, SCF, etc....)

Exercises will deal with simple runs and basic execution. The user should get familiar with the main inputs that have to be controlled/changed in typical SIESTA runs. User should also get acquainted with the fact that there are many other parameters for which reasonable default values are assumed, but may eventually be changed.

A. García

Pseudopotentials

A. García

How to generate and test pseudopotentials

D. Sanchez-Portal

Atomic orbitals of finite range as a basis set: why are they useful and how to generate them

J. Junquera

Code structure: calculation of the matrix elements of H and S and direct diagonalization

Exercises will deal with the generation and test of norm-conserving pseudopotentials, the use of different basis sets and how this affects the final results.

P. Ordejón

Order-N solvers: when and how to use them

D. Sanchez-Portal

Systematic convergence of realistic projects (Part I)

Systematic convergence of realistic projects (Part II)

P. Ordejón

Geometry optimization, molecular dynamics and vibrational spectra

D. Sanchez-Portal

Calculation of optical properties. Calculation of the macroscopic polarization in insulators

Exercises in this session will deal with the use of the linear scaling algorithms and molecular dynamics.

E. Anglada

Parallel SIESTA: compiling and running in parallel

J. Junquera

Analysis, visualization and postprocessing tools (Part I)

Analysis, visualization and postprocessing tools (Part II)

E. Anglada

How to get SIESTA

Exercises in this session will deal with the visualization of structures, the charge density, local density of states, wavefunctions, and other outputs of the program. If there is enough time we can also include exercises on the calculation of optical properties.

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JCNS Panel Meeting

November 29-30, 2007

The DIPC hosted the meeting of the JCNS Panel for proposals selection. After the permanent shut down of the research reactor FRJ-2 in Jülich, the *Jülich Centre for Neutron Science* (JCNS, <http://www.jcns.info>) has been founded. It encompasses the in-house research of the Institut für Festkörperforschung Jülich with neutrons, the instrument and method development and the instrument operation and user programs at the FRM-II reactor in Munich, the SNS Spallation Source in Oak Ridge and the ILL high-flux reactor in Grenoble. Twice a year, a committee of external experts in neutron scattering selects the best proposals from those submitted from all over the world to grant beam-time in the different instruments. The November meeting took place at the DIPC.

The Panel consisted of a Chairperson (A. Arbe, CFM, San Sebastián) and 8 members (Stephan Förster, Jean-Pierre Gaspard, Kim Leffmann, Roland May, Julian Oberdisse, Frederic Ott, Christian Pfeiderer and Dimitris Vlassopoulos). In addition, three representative persons from JCNS (Thomas Gutberlet, Sasha Ioffe and Reiner Zorn) attended the meeting to inform the Panel about the state of the art and future development of the instruments.

Universal Aspects in Soft Matter: Slow Dynamics

December 12-13, 2007

In the spirit of SoftComp, looking for universal features of different classes of soft materials is one of the major goals. This is an inter-area (topical) workshop with discussions of the properties of the slow dynamical processes taking place in different systems including polymers, colloids, biological molecules, micelles, liquid crystals. The main properties of the dynamics related to the glass transition, functionality of proteins yielding mechanism, reptation in polymers of different architectures, ageing etc. were addressed. A very rich variety of systems and phenomena were considered. Also noteworthy was the number of experimental techniques involved in the papers presented (dielectric and mechanical spectroscopy, NMR, neutron scattering, tracer diffusion, dynamic light scattering including novel developments with laser-speckle imaging, microscopy). From a theoretical point of view, the tremendous progress made in the last few years in this direction was obvious as well. We can say that the workshop was very worthwhile, giving a broad idea of the state of the art of this subject in the different areas of SoftComp.

CONTRIBUTIONS

J. Colmenero
Opening and Welcome

N. F. Fatkullin
NMR, the Corset effect and dynamics of polymer melts

A. Moreno
Entangled-like chain dynamics in non-entangled polymer blends with Large dynamic asymmetry

L. Dahbil
SANS observation of the relaxation of a hyperbranched polymer in a linear matrix after a large step strain deformation

M. Fuchs
Structural and conformational dynamics of supercooled polymer melts

P. Pfeiderer
Glassy dynamics in suspensions of hard ellipsoids

P. Schurtenberger
Clusters, viscoelastic phase transitions and glasses in protein solutions

R. Biehl
Global dynamics of the protein alcohol Dehydrogenase

S. Harris
Modeling the mechanics of duplex DNA

- E. Zaccarelli
Glasses in starts polymer mixtures (tentative)
- J. Stellbrink
Mesoscopic dynamics of star-like micelles
- B. Loppinet
Dense solutions of diblock copolymers multiarm stars: structure and dynamics
- J. K. G. Dhont & K. Kang
Tracer diffusion in isotropic and nematic colloidal rod networks: electrostatic interactions and hydrodynamic screening
- D. Vlassopolous
Towards a phenomenological description of yielding mechanisms in colloidal glasses
- F. Scheffold
Heterogeneous slow dynamics in a drying colloidal thin film
- J. Baschnagel
Structural relaxation in glass forming polymer films with one free surface
- D. Long
Case-II diffusion and solvent-polymer films drying: a meso-scale model
- W. Paul
Single molecule probes of the glass transition in polymer melts: a molecular dynamics investigation
- D. Cangialosi
Cooperative dynamics in non-polymeric glass-formers
- L. Ramos
Origin of the slow dynamics and the aging of a soft glass
- M. Cloitre
Slow dynamics and ageing in the rheology of soft concentrated dispersions
- C. Genix
Direct microscopic observation of structural relaxation in systems with tunable dynamic asymmetry
- C. Lorthioir
Dynamic heterogeneities in polymer/clay and polymer blend/clay nanocomposites: A solid state NMR investigation

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On December 14th, the Network Coordination Committee of the Network of Excellence SoftComp met at the DIPC. The aim was to define the activities of the different areas of the Network for the first six months of 2008 and give a first impulse to the organization of the next International Conference on Soft Matter, to be held in Granada in 2010.

The participants were: Dieter Richter (General Coordinator), Gerhard Gompper, Jan Dhont, Patricia Bassereau, Juan Colmenero, Massimo Noro, Dimitris Vlassopoulos, Luis Liz-Marsan, Katharina Schwemmer, Peter Olmsted, Hugo Bohn and Roque Hidalgo.