

# Insight



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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.

### CONTRIBUTIONS

J.-P. Bourgoin (CEA Saclay, France)

**Carbon Nanotubes based Nano-Electro-Mechanical Systems**

J. Gómez (Universidad Autónoma de Madrid, Spain)

**Tuning the conductance of single walled carbon nanotubes by ion irradiation in the Anderson localization regime**

J.J. Palacios (Universidad de Alicante, Spain)

**Schottky in Gold- and Palladium-contacted semiconducting carbon nanotubes**

M. Brandbyge (Technical University of Denmark)

**Transport in molecules and nanowires from density functional theory**

M. Szymonski (Jagiellonian University, Poland)

**Metal nanostructures assembled st semiconductor surfaces for anchoring and communication in molecular devices**

J.R. Galán Mascaros (ICMol, Spain)

**Magnetic and conducting molecular materials**

E. Ortega (Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain)

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

E. Meyer (Universität Basel, Switzerland)

**Force Microscopy Investigations Of Molecules**

M. Dubois (CEA-DRFMC, France)

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

P. Ordejon (ICMAB-CSIC, Spain)

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

L. Grill (Freie Universität Berlin, Germany)

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

M.T. González (Universität Basel, Switzerland)

**Break junctions in liquid for molecular electronics**

J. Veciana (ICMAB-CSIC, Spain)

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

T. Linderoth (Aarhus Universitet, Denmark)

**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

#### CHAIRMAN

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Prof. Richard M. Martin (University of Illinois, USA)

Prof. Manuel Martin-Lomas (CSIC, Spain)

Prof. Sir John B. Pendry (Imperial College London, United Kingdom)

**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.

#### CONTRIBUTIONS

**Nanophotonics** Chair: Prof. Clivia Sotomayor (Tyndall National Institute, Ireland)

M. Wegener (Universität Karlsruhe, Germany)

**Photonic metamaterials: Optics starts walking on two feet**

G. Badenes (ICFO-The Institute of Photonic Sciences, Spain)

**Nanophotonic devices and techniques for sensing applications**

N. Halas (Rice University, Texas, USA)

**Plasmonic nanostructures from artificial molecules to active nanodevices**

X. Zhang (University of California Berkeley, USA)

**Photonic metamaterials: Nano-scale plasmonics and super lens**

P. Nordlander (Rice University, Texas, USA)

**Plasmonic substrates for surface enhanced spectroscopies**

B. Wood (Imperial College London, United Kingdom)

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

**Nanostructures** Chair: Prof. Peter Nordlander (Rice University, Texas, USA)

U. Landman (Georgia Institute of Technology, USA)

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

J.B. Pethica (Trinity College Dublin, Ireland)

**Mechanics at single atoms & nanoimprint for lithography**

F. Briones (Instituto de Microelectrónica de Madrid-CNM-CSIC, Spain)

**Device integration of semiconductor and magnetic nanostructures**

N. Pascual (Berlin, Germany) Pascual José Ignacio Freie Universitet Berlin???

**Microscopy, spectroscopy and manipulation of single molecules and nanostructures**

**Management and Coordination** Chair: Prof. Pedro M. Echenique (UPV/EHU, DIPC, Spain)

G. Prentice (National Science Foundation, Virginia, USA)

**Nanoscale Science and Engineering at the NSF**

C. Sotomayor (Tyndall National Institute, Ireland)

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

J. Ahopelto (VTT Micro and Nanoelectronics, Finland)

**Emerging Nanopatterning methods: The research work of the EU Integrated Project NaPa**

**Nanostructures** Chair: Dr. Włodzimierz Jaskolski (Nicholas Copernicus University, Poland)

P. Hawrylak (Institute for Microstructural Sciences, National Research Council Canada)

**Nanoscale semiconductor structures**

J. Nelson (Imperial College London, United Kingdom)

**Nanostructured and molecular materials for photovoltaic energy conversion**

E. Muñoz (Instituto de Carboquímica, CSIC, Spain)

**Multifunctional carbon nanotube composite fibers**

D.S. Galvão (University of Campinas-São Paulo, Brazil)

**Nanowires and suspended atomic chains from Au-Ag alloys**

**Nanobiotechnology** Chair: Prof. Manuel Martin-Lomas (CSIC, Spain)

D. Wechsler (VDI Technologiezentrum GMBH, Germany)

**Perspectives of controllable nanoparticles in diagnosis and therapy**

S. Penadés (IIQ-CSIC, Spain)

**Biofunctional nanoparticles**

M.Vélez (Universidad Autónoma de Madrid, Spain)

**Biofunctionalized surfaces to study membrane bionanomachines**

M. García-Parajó (Institute for Bioengineering of Catalonia, Universitat de Barcelona, Spain)

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

G. Chirico (Università degli Studi di Milano, Italy)

**Voltage regulation of single molecule fluorescence**

Video Projection introduced by I. Schuller (University of California, San Diego, USA)

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

E. Artacho (University of Cambridge, United Kingdom)

**Ab initio calculations of nanostructured materials**

F.J. García de Abajo (Instituto de Óptica, CSIC, Madrid, Spain)

**Advances towards surface-state nanoelectronics**

J. Alonso (Universidad de Valladolid, Spain)

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

R. Miranda (Universidad Autónoma de Madrid, Spain)

**Self-organized nanomagnets and organic molecules at surfaces**

E. Ortega (Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain)

**One-dimensional quantum wells in noble metal surfaces and nanostructures**

W. Jaskolski (Nicholas Copernicus University, Poland)

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

K. Henson (IBM Microelectronics, New York, USA)

**CMOS trends for the Nanotechnology era**

F. Gámiz (Universidad de Granada, Spain)

**Electron transport in silicon based nano-transistors**

R. Rurali (Universitat Autònoma de Barcelona, Spain)

**Electronic and scattering properties of dopants in silicon nanowires**

I. Schuller (University of California, San Diego, USA)

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

A. Hernando (Instituto de Magnetismo Aplicado, Universidad Autónoma de Madrid, Spain)

**Orbital magnetism in Au and ZnO nanoparticles**

D. Petit (Imperial College London, United Kingdom)

**Magnetic logic devices for ultra high density data storage**

F. Castaño (Massachusetts Institute of Technology, USA)

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

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## Confinement: Universal Aspects in Soft Matter

December 12-13, 2006

### ORGANIZER

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

**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.

### CONTRIBUTIONS

J. Colmenero (Universidad del País Vasco/Euskal Herriko Unibertsitatea, DIPC, CSIC, Spain)  
**Why Confinement?**

F. Kremer (University of Leipzig, Germany)  
**Molecular dynamics of thin polymer layers.**

R. Zorn (Forschungszentrum Jülich, Germany)  
**Effect of nanoscopic confinement on the dynamics of glass-forming liquids and polymers.**

D. Schwahn (Forschungszentrum Jülich, Germany)  
**Effect of asymmetric Component Mobility on Thermal Composition Fluctuations in the PEO/PMMA Blend.**

M. Tyagi (Donostia International Physics Center, Spain)  
**Dynamic confinement effects in a blend of poly(ethylene oxide) with poly(vinyl acetate).**

P. Lang (Forschungszentrum Jülich, Germany)  
**Colloidal Dynamics close to Walls.**

V. Krakoviack (École normale supérieure de Lyon, France)  
**Slow dynamics in confinement: A mode-coupling theory.**

A. Moreno (Donostia International Physics Center, Spain)  
**Confinement in simple binary systems with and without connectivity.**

W.J. Briels (University of Twente, The Netherlands)  
**Coarse graining of slow variables applied to star-polymers.**

M. Oettle (Johannes Gutenberg-Universität Mainz, Germany)  
**Effective colloidal interactions at fluid interfaces.**

H. Frielinghaus (Forschungszentrum Jülich, Germany)  
**Confinement effects of block copolymers in bicontinuous microemulsions.**

S. Cervený (Donostia International Physics Center, Spain)  
**Confinement effects in water/polymers and water/biopolymers systems.**

P. Moldenaers (K.U. Leuven, Belgium)  
**Effect of confinement on droplet dynamics in two-phase polymer blends.**

P. Moreau (Centre de Recherche Paul Pascal, Bordeaux, France)  
**Confinement effect on structural and dynamical properties of a doped and oriented lamellar phases.**

D. Cangialosi (Donostia International Physics Center, Spain)  
**Confinement and cooperativity of the alpha relaxation in glass forming polymers.**

B. Loppinet (FORTH, Institute of Electronic Structure & Laser, Greece)  
**Confinement effects investigated by dynamic light scattering.**

R. Lund (Donostia International Physics Center, Spain)  
**Dynamics of Polymers Confined in a Micellar Core.**

J. Martín (CSIC, Instituto de Ciencia y Tecnología de Polímeros, Madrid, Spain)  
**Nanoporous Anodic Alumina as confining medium for polymers.**

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 M. Tyagi ..... Donostia International Physics Center, Spain  
 E. van Ruymbeke ..... FORTH, Institute of Electronic Structure & Laser, Greece  
 D. Vlassopoulos ..... FORTH, University of Crete, Greece  
 L. Willner ..... IFF-FZ, Forschungszentrum Jülich, Germany  
 R. Zorn ..... IFF-FZ, Forschungszentrum Jülich, Germany



## 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

## ORGANIZING COMMITTEE

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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<sub>0.3</sub>MoO<sub>3</sub>

## 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 N<sub>2</sub> 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<sub>1-x</sub>Ge<sub>x</sub> 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

U. Heinzmann

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

A. Vazquez de Parga

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 Al<sub>2</sub>O<sub>3</sub>

H. van Beijeren

Finite size effects on equilibrium shapes due to line tensions

**Ion Surface II** Chair: J.R. Manson

F. Aumayr

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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 V. Etxebarria ..... UPV/EHU, Leioa, Spain  
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 J. Campo ..... CSIC, Spain

J. Doncel ..... Ministry of Education and Science, Spain

C. Oyón ..... Basque Government  
 A. Ansuátegui ..... Basque Government

#### Representatives from companies:

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 J. Alonso ..... TEKNIKER, Spain  
 I. Quintana ..... TEKNIKER, Spain  
 M. Carrera ..... AVS, Spain  
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## Ab-initio Approaches to Electron-phonon Coupling and Superconductivity

May 28-30, 2007

### ORGANIZERS

**Prof. Ole K. Andersen** (Max-Planck-Institute for Solid State Research, Stuttgart, Germany)

**Prof. Eugene V. Chulkov** (Universidad del País Vasco/Euskal Herriko Unibertsitatea and Donostia International Physics Center, Spain)

**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 MgB<sub>2</sub>

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 Li<sub>2</sub>B<sub>2</sub>

S. Massidda

Impurity effects in superconductivity of MgB<sub>2</sub>

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 SrTiO<sub>3</sub>

O. Gunnarsson

Many-body effects in electron-phonon coupling

O. Fischer

Electron-phonon interaction in Chevrel-type compounds

A. Goldoni

Band dispersion K<sub>6</sub>C<sub>60</sub>(110) and K<sub>3</sub>C<sub>60</sub>(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: CaC<sub>6</sub> and SrC<sub>6</sub>

J. Kunes

KOs<sub>2</sub>O<sub>6</sub>: 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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 C. Bersier .....Freie Universität Berlin, Germany

## 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.

## CONTRIBUTIONS

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## Elementary Reactive Processes at Surfaces

August 30-September 1, 2007

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**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 CO<sub>2</sub> 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

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TDDFT simulations of electronic energy dissipation during chemisorption

C. Carbogno

Spin effects in the adsorption of O<sub>2</sub> on Al(111) surfaces

G. Darling

Surface temperature effects in reactive dynamics

B. Jackson

The role of surface reconstruction in gas-surface reactions

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Multidimensional "high level" calculations for a prototype system: H<sub>2</sub>/Cu(111)

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Sticking probability of N<sub>2</sub>/W(110) using different exchange correlation functionals

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

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Dissociative adsorption of H<sub>2</sub> 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
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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. Guillelot  
Nanostructure formation by reaction of H<sub>2</sub>O with pre-adsorbed O on a Ag(110) surface
- P. Cabrera-Sanfélix  
Adsorption of H<sub>2</sub>O and CO<sub>2</sub> at the surface of atmospheric particles
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Fast and across steps: Hydrogen diffusion on Si(001) under unusual conditions
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The influence of steps on dissociative adsorption of H<sub>2</sub> on Pt(111)
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Density functional theory calculations for the Hydrogen evolution reaction in an electrochemical double layer on the Pt(111) electrode
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Hydrogen atom clustering and molecule formation on graphitic surfaces
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Quantum studies of Hydrogen dynamics on graphite surfaces
- C. Arasa  
Kinetics and dynamics study of the Oxygen Eley-Rideal reaction on  $\beta$ -cristobalite (100) surface
- P. Larregaray  
On the validity of semi-classical statistical theories of chemical reactions: From triatomic to gas-surface elementary processes
- V.V. Petrunin  
Use of electronic excitation to initiate and control elementary chemical reactions on gas-surface interphase
- J. Cerdón  
Engineering electron bands in dislocation networks
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The reactivity of Ni nanostructures on stepped Rh surfaces

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## TNT2007

September 3-7, 2007

## SPONSORS

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**TNT2007 is been launched following the overwhelming success** of earlier Nanotechnology Conferences. The TNT2007 edition (September 03-07, 2007) will be held in the Kursaal congress facilities (San Sebastian, Spain). This high-level scientific meeting series aims to present a broad range of current research in Nanoscience and Nanotechnology as well as related policies (European Commission, etc.) or other kind of initiatives (iNANO, FinNano, GDR-E, etc.). TNT events have demonstrated that they are particularly effective in transmitting information and establishing contacts among workers in this field. The TNT2007 structure will keep the fundamental features of the previous editions, providing a unique opportunity for broad interaction

## CONTRIBUTIONS

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**Self-Organization of Functional Supramolecular Devices**

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**Supermolecules as soft materials with dynamic structures and functions in all dimensions: from molecules to nano, micro, and bulk**

S. Biswas (Indian Institute of Science, India)

**Frictional dissipation in self assembled MONOLayers of organic molecules**

W. Hofer (University of Liverpool, United Kingdom)

**Perfect ordering of molecular nanostructures**

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F. Besenbacher (iNANO, Denmark)

**Enhanced Bonding of Gold Nanoparticles on Oxidized TiO<sub>2</sub>(110)**

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**Probing reaction dynamics at metal surfaces with H<sub>2</sub> diffraction**

Chair: F. Besenbacher (iNANO, Denmark)

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**High flexibility of DNA on short length scales probed by atomic force microscopy**

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**Bacterial protein crystals as pure biomimetic nano-molecules**

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**Obtaining information at the molecular level with mesoscopic fluorescent measurements**

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**Electronic transport in single-molecule junctions**

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**Single Molecular Devices**

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**Tuning the conductance of a molecular switch**

D. Porath (The Hebrew University of Jerusalem, Israel)

**Scanning tunneling spectroscopy and polarizability measurements of DNA and G4-DNA molecules**

S. De Franceschi (CEA/DRFMC, France)

**Electron transport in semiconductor nanowires**

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**Metallic Nanowires: When is an alloy not an alloy ?**

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**Nuclear-spintronics in semiconductor nanostructures**

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**Nanospintronics meets relativistic quantum physics: Ubiquity of Zitterbewegung effects**

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**Nuclear spin detection enabled by ultra-sensitive cantilevers**

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**Chemical identification of individual surface atoms using dynamic force microscopy**

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**Scanning Tunnelling Microscopy in a Microampère Range**

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**Electrostatic Force Microscopy of InGa at Cryogenic Temperatures**

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**Adatom-adatom interaction mediated by an underlying surface phase transition**

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**Magnetic resonance force microscopy: the quest for a molecular structure microscope**

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**Magnetic properties of ZnO Nanoparticles**

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**Magnetism in Gold Nanoparticles and Gold clusters: The Role of Chemisorption and Size**

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**Challenges and Opportunities in Nano-Magnetism Research and Technology**

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**Interface and composition effects determining the magnetic properties of bi-metallic nanostructures**

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**Breaking Abbe's barrier: Diffraction-unlimited resolution in far-field microscopy**

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**Nano-antennas - Tools for light on the nanoscale**

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**Scattering-type Near-Field Microscopy: From Nanoscale Infrared Material Recognition to Superlens Studies**

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**Controlling the Nanoscale: From Nanocatalysis to Nanowires, DNA Damage, and Wigner Molecules**

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**AC Josephson effect and resonant superconducting transport through vibrating Nb nanowires**

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**Atomic, Electronic, and Transport Properties of semiconducting and molecular wires and their metallic Contacts**  
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**Boron Nitride Nanomesh: Functionality from a Corrugated Monolayer**

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**Ballistic to diffusive crossover in the sliding of kicked clusters**  
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**Nanocluster DFT studies with applications to production and storage of hydrogen**  
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**Computer simulations of nanopatterning**  
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**Atomistic modeling of metal/high-k oxide interface properties as function of gas treatment**  
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**Predicting the properties of new oxides for nano-devices**  
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**Simulation of atomic scale statistical variability in nano-CMOS devices using DD, MC and QT simulation techniques**

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**Transformation Optics: Designing Optics on the Nanoscale**  
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**A novel low energy collective excitation at metal surfaces**  
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**Making lasers from dust: The physics and applications of random lasers**  
 R. Carminati (Ecole Centrale Paris, France)  
**Local density of states in near-field optics**

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**Nanoplasmonics – from fundamental studies to novel functionalities**  
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**Photoluminescent diamond nanoparticles**

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**The Puzzling Behavior of Liquid Water: Some Clues from the Nanoscale**  
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**Hydrated ions as nano-ball-bearings**  
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**Biological Water**  
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**Nanofabrication of inorganic functional structures by protein supramolecules**  
**WET-NANOTECHNOLOGY**

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**Revisiting Charge Transport at the Mesoscopic Scale : Emerging quantum phenomena in the light of advanced Computational Approaches**  
 G. Lanzani (Politecnico di Milano, Italy)  
**Dynamics at the nanoscale: Ultrafast Exciton processes in Single Wall Carbon Nanotubes**

B. Hernandez Juarez (Institute of Physical Chemistry, Germany)  
**Quantum dot attachment and morphology control by carbon nanotubes**  
 A. Rycerz (Jagiellonian University, Poland)  
**Valley filter and valley valve in graphene**  
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**Science and Nanotechnology of Nano-carbon materials**

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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.