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## First Symposium of the nanoICT Coordination Action

February 26, 2008

### ORGANIZERS

Antonio Correia (Fundación Phantoms, Spain)

Daniel Sanchez Portal (CSIC-UPV/EHU, DIPC, Spain)

Nanoelectronics represent a strategic technology considering the wide range of possible applications. These include telecommunications, automotive, multimedia, consumer goods and medical systems. In the semiconductor industry, Complementary Metal Oxide Semiconductor (CMOS) technology will certainly continue to have a predominant market position in the future. However, there are still a number of technological challenges, which have to be tackled if CMOS downscaling should be pursued until feature sizes will reach 10 nm around the year 2015-2020. This miniaturization will offer opportunities for alternative nanodevices (biomolecular-based technologies and nanomechanics) to be incorporated into CMOS platforms providing an increasing diversification of functions.

The EC policies aiming at maintaining Europe at the forefront of the Information Society, through investment in the future key domains or aiming at optimising the development and diffusion of emerging technologies are clearly within the scope of the recently launched nanoICT Coordination Action (CA). High-level dissemination activities within nanoICT CA 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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### CONTRIBUTIONS

Antonio Correia (Fundación Phantoms, Spain)

**nanoICT Coordination Action**

Henri Jaffrès (CNRS/Thales, France)

**Spin injection in semiconducting nanostructures and heterostructures: issues and perspectives**

Marek Szymonski (Jagiellonian University, Poland)

**Anchoring and LT-STM/STS characterization of single organic molecules at semiconducting and insulating surfaces**

Ricardo Díez-Muiño (CSIC-UPV/EHU, Spain)

**Non-adiabatic effects in the reactivity of molecules at metal surfaces**

Guillermo Villanueva (EPFL, Switzerland)

**MEMS & Nanotechnology**

Bill Milne (University of Cambridge, UK)

**Carbon Nanotubes- the future of Electronics?**

Robert Baptist (CEA-LETI, France)

**Nanoscience & Nanoelectronics at CEA**

Andres Arnau (DIPC / EHU-UPV, Spain)

**Formation of dispersive hybrid bands at an organic-metal interface**

Clivia Sotomayor Torres (Tyndall Institute, Ireland & ICN, Spain)

**Nanophotonics in the European Research Area: the PhOREMOST perspective**

Number of participants: 34

## Ultrafast2008

### International Symposium

Electron dynamics and electron mediated phenomena at surfaces: femto-chemistry and atto-physics

May 7-8, 2008

### ORGANIZERS

Raimundo Pérez-Hernández and Juan A. González-Palomino (Fundación Ramón Areces, Spain)

Pedro M. Echenique and Daniel Sanchez Portal (DIPC, Spain)

The UltraFast2008 workshop was co-organized by the Ramon Areces Foundation and DIPC. The symposium took place at DIPC and gathered a relatively small and selected group of scientists working in the field of electron dynamics and related subjects. The focus was mainly on the implications of the dynamical processes to the basic understanding of the physics and chemistry of materials and, in particular, of surfaces. Some lectures on the state of the art in fast time-dependent processes in atoms and molecules were also included. The aim of this high-level scientific meeting is to debate about the current status of the field, new perspectives and hot topics, and the basic physics underlying observed phenomena. Some important open questions are: Can chemical and biological reactions be steered by controlling electronic motion on molecular orbitals? How does radiation damage biological systems? What are the most effective ways to excite atoms and molecules to highly excited states and how this excitation and the subsequent decay processes can be influenced by electromagnetic fields? Can electromagnetic fields be used to influence the flow of electrons in nanometer scale electronic devices? Will this open a route for a faster operation of electronic devices?

### Attophysics and femtochemistry

Attophysics and femtochemistry are the sciences of electrons in motion. Electrons in motion carry electronic current, emit electromagnetic waves, create or destroy molecules, and cause radiation damage in biological systems. Consequently, they are key players in information, industrial, and medical technologies and physical, chemical, and life sciences likewise. In integrated circuits their motion switches current and voltage within picoseconds. In molecules electrons form chemical bonds. On being excited they can trigger chemical and biochemical reactions within femtoseconds. Their oscillatory motion in atoms with a period of 1-2 femtoseconds or less is responsible for emission of visible, ultraviolet, and x-ray light. Electrons travel relevant distances in atoms, molecules, and nanometer-scale semiconductor structures in tens to thousands of attoseconds. Obtaining a detailed in-sight into this motion and gaining the ability to control it will have important implications for many fields of science. Speeding up electronics, steering chemical/biochemical reactions, developing sources of laser-like ultraviolet and x-ray light, and better radiation therapies most likely constitute only a minority of future implications.

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### CONTRIBUTIONS

Dr. Adrian L. Cavalieri (Max-Planck-Institut für Quantenoptik, Germany)

**Attosecond physics**

Prof. Dr. Ulrich Heinzmann (Universität Bielefeld, Germany)

**Attosecond time-resolved photoemission on metal surfaces**

Prof. A. K. Kazansky (V.A. Fock Institute of Physics, Saint-Petersburg State University, Russia)

**Some computations for the attosecond streaking experiments**

2008

2008

2008

Prof. Dr. Wilfried Wurth (University of Hamburg, Germany)

X-ray spectroscopic methods to study dynamical processes in materials

Prof. Dr. Helmut Zacharias (Physikalisches Institut Westfälische-Wilhelms Universität, Germany)

Electron dynamics at surfaces at high photon energies using the XUV Free Electron Laser (FLASH)

Prof. Dr. Hrvoje Petek (University of Pittsburgh, USA)

Ultrafast photoemission electron microscopy: Imaging light with electrons on femto/nano scale

Prof. Andrey G. Borissov (Université de Paris-Sud, France)

Electron propagation along Cu nanowires on Cu(111) surface

Prof. Branko Gumhalter (Institute of Physics, Zagreb, Croatia)

Ultrafast electron dynamics in surface bands

Prof. Dr. José Ignacio Pascual (Freie Universität Berlin, Germany)

Electron dynamics at metal surfaces "visualized" with STM

Dr. Jörg Kröger (Christian-Albrechts-Universität zu Kiel, Germany)

Conductance of single atoms and molecules in a low-temperature STM

Prof. Dr. Hans-Joachim Freund (Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany)

Structure, morphology and electronics of nanoparticles on oxide surfaces

Prof. Dr. Martin Wolf (Free University Berlin, Germany)

Ultrafast dynamics of photo-induced processes at interfaces probed by time-resolved photoelectron spectroscopy

Prof. Dr. W. Pfeiffer (Universität Bielefeld, Germany)

Spatio-temporal control of nanoptical fields

Prof. Dr. Martin Weinelt (Max Born Institute, Berlin, Germany)

Hot spots and spin waves

Prof. Dr. Thomas Fauster (Universität Erlangen-Nürnberg, Germany)

Scattering of electrons in image-potential states

Prof. Dr. Ulrich Höfer (Philipps-Universität Marburg, Germany)

Dynamics of image-potential resonances

Prof. Dr. Mark I. Stockman (Georgia State University, USA)

Ultrafast, and Quantum Nanoplasmonics

Dr. Tadaaki Nagao (National Institute for Materials Science, Japan)

Atom-scale plasmonics: molding plasmons into atom chains and atoms sheets

Prof. Dr. Dietrich Menzel (TU München, Germany)

Photochemistry at metal nanoparticles

Prof. Dr. W. Eberhardt (BESSY, Berlin, Germany)

Real-time Evolution of the Valence Orbitals in a Dissociating Molecule Revealed by Femtosecond Photoelectron Spectroscopy

Prof. Dr. Reinhard Doerner (Institut für Kernphysik, Germany)

Ultrafast Probing of Core Hole Localization in Diatomic Molecules

Prof. D. R. Herschbach (Harvard University, USA)

Electron Dynamics in Surface Chemistry

Number of participants: 41

## Quantum Coherence and Controllability at the Mesoscale

May 12-23, 2008

ORGANIZING COMMITTEE

Boris L. Alschuler (Columbia University, New York, USA)

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

Vladimir I. Falko (Lancaster University, UK)

Francisco Guinea (ICMM-CSIC, Spain)

CONTRIBUTIONS

Carlo Beenakker

Shot noise in graphene

Xavier Waintal

Do metals exist in two dimensions? A study of many-body localization in high mobility Si MOSFETs

Thierry Giamarchi

Low dimensional systems and cold atomic gases

Alejandro Muramatsu

Nonequilibrium dynamics of strongly correlated quantum gases

Mark Raizen

Generation of few-body atomic number states towards scalable entanglement

Fernando Sols

Andreev reflection in bosonic condensates

Gora Slyapnikov

Anderson localization of evolving Bose-Einstein condensates

Natan Andrei

Quantum impurities out of equilibrium

Massimo Inguscio

Anderson localization of ultra-cold atoms in random lattices

Eugene Demler

New route to supersolid phases: dipolar interactions in spinor condensates

Ehud Altman

Probing non local order parameters in highly correlated Bose insulators

Oleksiy Kashuba

AMR and ATP in ferromagnetic alloys

Konstantyn Kechedzhi

Magneto-phonon resonance in graphene

Andre Geim

Graphene update

Eva Andrei

Scanning Tunneling Microscopy and transport experiments on graphene

Adrian Batchtold

Nanotube & Graphene Electro-Mechanics

Leonid Levitov

Conformal Invariance and Conductance of graphene

Pablo Jarillo-Herrero

2008

2008

Electronic transport in graphene nanostructures

Antonio Castro-Neto

A few topics in graphene physics

Mikhail Katsnelson

Scattering mechanisms and charge carrier transport in graphene

Luis Brey

Charged inhomogeneities in rippled graphene and diluted graphene antiferromagnet

Tilman Esslinger

Cavity QED with a BEC and a Mott insulator of Fermions

José Carmelo

Coherent and incoherent pairing in a square-lattice quantum liquid

Masahito Ueda

Symmetry breaking of Bose-Einstein condensates with internal degrees of freedom

Leonid Glazman

1D Fermions and Bosons beyond the Luttinger Liquid picture

Alex Kamenev

Generating dark solitons by single photons

Wolfgang Schleich

Gauss sums and factorization of numbers

Yuki Kawaguchi

Knot Soliton in a Spinor BEC

Yuval Gefen

Weak Measurements in Solid State

Gerd Schön

Decoherence and Relaxation in Driven Circuit QED systems

Yuri Galperin

Non-Gaussian decoherence in qubits due to low-frequency noise

Alexander Tartakovskii

Nuclear spin effects in optically pumped semiconductor quantum dots

Enrique Louis

Transport through organic molecules containing magnetic atoms: effects of symmetry and Coulomb interaction

Baruch Horovitz

The dephasing scenario of a particle on a ring with dissipative environments

Nicolas Agrait

Ultralong natural graphene nanoribbons

Maria Vozmediano

Topological disorder, curvature, and minimal conductivity in graphene

Marco Polini

Pseudospintronics with semiconductors and graphene bilayers

Number of participants: 50

## 1st DIPC-nanoGUNE-ICFO Meeting

May 20, 2008

This meeting is the first encounter between research teams at ICFO, DIPC and nanoGUNE to obtain first hand information about ongoing research projects and explore possible collaborations on specific projects dealing mainly with nanophotonics.

A main topic of research, both at ICFO and DIPC, is related to the study of optical antennas for sensing and enhanced fluorescence. Teams of both institutes gave presentations on this topic and explored possible collaborations for further research on nanoantennas.

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### CONTRIBUTIONS

P. M. Echenique

Acoustic plasmons

N. Van Hulst

Molecular nanophotonics

J. Aizpurua

Plasmonic nanoantennas

H. Petek

Ultrafast photoemission electron microscopy: Imaging light with electrons on femto/nano scale

G. Badenes

Nanophotonic devices

E. Ortega

Tuning electronic states in self-assembled metallic superlattices

R. Hillenbrand

Near-field nanoscopy

J. Martorell

Non-linear nanophotonics

D. Sanchez Portal

Electronic structure from first principles

R. Quidant

Plasmon nano-optics

T. Pitarke

nanoGUNE: The big challenge of the small

Number of participants: 12

2008

## New Frontiers in Magnetism

September 22, 2008

### ORGANIZERS

Pepa Cabrera Sanfelix (DIPC, Spain)

Pedro M. Echenique (DIPC and CSIC-UPV/EHU, Spain)

DIPC hosted a meeting of leading researchers in the field of Magnetism. The purpose of this symposium was to acknowledge Professor Agustin Del Moral's contribution to science and celebrate the recent publication of his book *Handbook of Magnetostriction and Magnetostrictive Materials*. The goal of the meeting was to bring together researchers actively working in any field related to magnetism, particularly low dimensional systems, and discuss recent results and the future perspectives.

2008

### CONTRIBUTIONS

A. Howie

Time and Frequency - the new Frontiers in Microscopy

F. Yndurain

Magnetism in low dimensional systems

A. Berger

Controlling Granular Magnetic Materials on the Nano-Scale

M. J. Azanza

Magnetic Field Effects on Neurones

D. Sánchez-Portal

Magnetism of graphene substitutionally doped with transition metals

A. Ayuela

Magnetic Induced Shape-Memory Alloys

L. Panina

Adaptive Metamaterials Based on Ferromagnetic Wires

A. Hernando

Microwave attenuation induced by metallic microwires embedded in a dielectric matrix

F. Flores

A new N-fold degenerate model for transition metal single atom Kondo resonances

P. M. Echenique

Electron Dynamics at Surfaces

A. Del Moral

Speech about the book: "Handbook of Magnetostriction And Magnetostrictive Materials"

Number of participants: 14

## Workshop on Bio-Inspired Photonic Structures

July 9-15, 2009

### ORGANIZING COMMITTEE

Jean-Pol Vigneron (University of Namur, Belgium)

Pedro Miguel Echenique (DIPC and CSIC-UPV/EHU, Spain)

Amand Lucas (University of Namur, Belgium)

Giorgio Benedek, (Università degli Studi di Milano, Italy)

Javier Aizpurua (CSIC-UPV/EHU, Spain)

This meeting, simultaneously a workshop and a summer school, will include tutorials and research seminars on the biological and physical aspects of photonic structures. It was organized in the splendid venue of the San Sebastian historic Miramar Palace. Established researchers and students from physics, chemistry, biology and engineering with a strong interest for interdisciplinary collaboration, were all welcome.

2009

The meeting covered many aspects of biophotonics: quantitative study of nanomorphology, optical properties, biological functions of colors, taxonomic search for species of interest, reverse engineered modelling and computer simulations, bio-mimetic devices, etc. The physical mechanisms involved in these structures are inspiring for device applications in material science and optical engineering.

### CONTRIBUTIONS

Andrew Parker Evolution's Big Bang- the Origin of Optics

Eli Yablonovitch Applications of Photonic Crystal Pigments in Technology

Doেকে Stavenга Vision and colors

Jacques Livage Pigmentary coloration

Jean-Pol Vigneron Physics of structural coloration

Andrew Parker Evolutionist's point of view

Richard Prum Optics and self assembly of amorphous photonic nanostructures in birds

Jacques Pasteels Animal defense strategies

Jian Zi Biological Photonic Crystal

Jacques Lafait Defining and measuring color

Serge Berthier Multiscale aspects of visual appearance

Michel Milinkovitch Molecular Phylogeny and Evo-Devo

Claus Nielsen Zoological systematics and classification

Cefe López Opal Structures

Gustaaf Van Tendeloo Electron microscopies

László Biró Bio-inspired artificial structures

Davy Galliot Composite organic—Inorganic Butterfly Scales: What Do We learn When Disorder Meets Order!

Claus Helix Nielsen Biomimetic membranes for separation and sensor applications

Number of participants: 66

# Summer School on Simulation Approaches to Problems in Molecular and Cellular Biology

August 31 - September 5, 2009

## ORGANIZING COMMITTEE

Paolo Carloni (SISSA and INFN DEMOCRITOS, Italy)

Michele Parrinello (ETH Lugano, Switzerland)

Ursula Rothlisberger (EPFL, Switzerland)

Daniel Sanchez Portal (CSIC-UPV/EHU, DIPC, Spain)

Angel Rubio (CSIC-UPV/EHU, Spain)

Cellular functions - like growth, (programmed) cell death, metabolism etc - ultimately depend of interactions between macromolecules encoded by DNA. Proteins and RNA directly control the cell and regulate its functions through the reactions they perform, by allosteric changes driven by endogeneous and exogeneous factors and by their mutual interactions. All of these processes involve molecular recognition, i.e. the process by which two or more biological molecules interact to form a specific complex. Molecular recognition is dominated by short-range, often transient, interactions at the contact surface of the interacting molecules. Even conformational changes and assembly of very large macromolecular aggregates, which can be propagated through long distances (tens of Angstroms), are the sum of local interactions between small molecules (like messengers) or macromolecules with their cellular targets.

Ultimately, therefore, even the understanding of the integration of biological complexes into cellular pathways (the so called 'systems biology') requires mechanistic understanding of the physical basis of molecular recognition. A quantitative description of cellular pathways in molecular terms is still mostly missing, although it would strongly impact on pharmaceutical sciences, as drugs target (and mutations affect) pathways, rather than single biomolecules. Such information is also crucial in nanobiotechnology, e.g. to design artificial sensing devices, which in Nature involve entire cascades of events and not only a single protein.

Molecular simulation constitute a key field to contribute to this issue. It can predict structure, dynamics, energetics, reactivity and spectroscopic properties of the cellular components (i.e. large macromolecular aggregates) involved in these pathways.

Tremendous challenges have to be taken before this ambitious goal can be reached. First, the systems are very complex and so are the interactions involved. In addition, ligand-protein processes involve small changes of free energies (less than 1 eV for non-covalent protein-protein interactions), and they are often entropy-driven. Next, the environment is very complex: cell membranes are far from being a simple lipid bilayer whilst the cytoplasm is far from being a simple aqueous solution. Finally, most often experimental structural information is partially or totally lacking.

## Scientific Objectives

The School's main goal is to present recent developments and applications of biomolecular simulation approaches aimed at predicting structure, dynamics and energetics of biomolecules. Aspects of bioinformatics-based structural prediction algorithms will be also presented.

Topics include:

Simulation of rare events

Prediction from first principles of spectroscopic and redox properties of biomolecules

Protein and nucleic acid structure prediction

Critical analysis of the force fields used for biomolecular simulation

Molecular simulation of cellular events

Simulation in molecular medicine

## CONTRIBUTIONS

Hutter Juerg (University of Zurich, Switzerland)

Progress in large scale density functional calculations

Calculation of NMR and EPR parameters for proteins in solution

Alber Frank (UCLA, Los Angeles, USA)

Determining the structures of macromolecular assemblies – Part 1

Determining the structures of macromolecular assemblies – Part 2

Voth Gregory A. (University of Utah, Salt Lake City, USA)

Rigorous coarse-graining of condensed phase and biomolecular systems

Multiscale modeling of proteins and membranes: from the molecular to the mesoscale

Cascella Michele (UNIBE, Bern, Switzerland)

Development of unbiased coarse grained potentials for simulations of proteins

Dal Peraro Matteo (EPFL Lausanne, Switzerland)

Coarse-grained electrostatics in multiscale simulations of proteins

Lavery Richard (Institut de Biologie et Chimie des Protéines, Lyon, France)

DNA dynamics and recognition

Coarse-grain models of protein mechanics

Orozco Modesto (Institute for Research in Biomedicine, Barcelona, Spain)

Pushing the boundary of MD simulations. Proteome scale atomistic simulations

Coarse grained dynamics simulations of proteins and nucleic acids

Sulpizi Marialore (University of Cambridge, UK)

Redox properties in metalloproteins

Pka calculations from DFT-based MD simulations

Dal Peraro Matteo (EPFL Lausanne, Switzerland)

Proton conduction and drug binding in the M2 channel from Influenza A virus

Cascella Michele (UNIBE, Bern, Switzerland)

Electronic structure/function relationship in copper-bound redox proteins

Gervasio Francesco (Fundacion CNIO - Carlos III, Madrid, Spain)

Quantitative structure-activity relationship with Metadynamics and Path-collective variables: ligand binding

Quantitative structure-activity relationship with Metadynamics and Path-collective variables: conformational selection and induced fold effects

Piana Stefano (D.E. Shaw Research, New York, USA)

The precision and accuracy problems in MD simulations

Improving force fields for MD simulations

2009

2009



Rubio Angel (ETSF, Donostia-San Sebastian, Spain)  
First principles description of the optical properties of biochromophores

Tavernelli Ivano (EPFL, Lausanne, Switzerland)  
TDDFT as a tool in chemistry and biology  
Light driven reactions in biological systems

Rovira Carme (ICREA, Barcelona, Spain)  
Substrate conformational changes in glycoside hydrolase catalysis  
The reaction mechanisms of heme peroxidases by QM/MM simulations

Grubmüller Helmut (MPI, Göttingen, Germany)  
Conformational motions of biological macromolecules  
Molecular dynamics simulations of biological nanomachines: may the force be with you

Raugei Simone (SISSA and INFN-DEMOCRITOS, Trieste, Italy)  
Computational vibrational spectroscopy for biomolecules: basics  
Computational vibrational spectroscopy for biomolecules: an application to the bacterial resistance to antibiotics

Guidoni Leonardo (Università degli Studi dell'Aquila, L'Aquila, Italy)  
Computing vibrational spectra of biomolecules by Quantum Mechanics/  
Molecular Mechanics simulations  
First principles calculations of photoreceptors

Participant Talks  
Brunk Elizabeth (EPFL, Lausanne, Switzerland)  
Zhu Lihze (University of Amsterdam, Amsterdam, The Netherlands)  
Valeria Losasso (SISSA, Trieste, Italy)  
Tipmanee Varomyalin (University of Cambridge, Cambridge, UK)  
Deplazes Evelyne (University of Western Australia, Crawley, Australia)  
Delemotte Lucie (Université Henri Poincaré, Nancy, France)

Number of participants: 48

## Workshop on Inorganic Nanotubes Experiment and Theory

September 2-4, 2009

### ORGANIZING COMMITTEE

Andrés Ayuela (CSIC-UPV/EHU, Spain)  
Pedro Miguel Echenique (DIPC and CSIC-UPV/EHU, Spain)  
Gotthard Seifert (TU Dresden, Germany)  
Jorge Sanchez-Dolado (NANOC-LABEIN Technological Center, Bilbao, Spain)

Nanotubes have attracted much attention of experimentalists and theorists. The informations about construction, synthesis and properties of the carbon nanotubes were published in numerous publications and books. At present, not only these new allotropes of carbon focus on fundamental research, but they find also its way in many applications.

Simultaneously with the discovery of the carbon nanotubes a question appeared — Can nanotubular structures be produced only based on carbon? The synthesis of the noncarbon nanotubes was realized in 1992 based on the molybdenum and tungsten disulphides. The hollow 1D nanostructures are not the exclusive phenomena for carbon, but they are possible for other compounds such as MoS<sub>2</sub> and WS<sub>2</sub>! During last 15 years the nanotubes of almost a dozen of inorganic compounds were discovered. Although the inorganic nanotubes were observed soon, one year after the carbon nanotubes, a systematic view on their synthesis, their properties and their potentials for applications is still very limited.

This workshop aimed to provide a forum for communication amongst scientists working in the field of Inorganic Nanotubes. Similar to the vast development on Carbon Nanotubes we hope to encourage the generation of new ideas for the development of novel nanotubular systems and their properties bringing together scientists working both experimentally and theoretically on Inorganic Nanotubes. The frame of the workshop was planned to be small to provide a productive scientific environment for interesting and exciting ideas.

The range of topics was rather broad and considered experimental as well as theoretical aspects on:  
Synthesis  
Structure and Characterization  
Mechanical Properties  
Electronic and Optical Properties  
Applications (tribological, catalysis, solar cells, etc.).

There was also a celebration for the 65th birthday of Prof. Reshf Tenne, who, since the discovery of inorganic nanotubes, has provided significant contributions and strongly influenced this field.

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### CONTRIBUTIONS

Reshef Tenne  
Update on selected topics related to inorganic nanotubes

Alexander Quandt  
Boron nanotubes- Theory, experiments, and applications

Julio A. Alonso  
Theoretical study of Boron and BeB<sub>2</sub> nanotubes

2009

2009

Janice L. Musfeldt  
Dynamical charge and structural strain in MoS<sub>2</sub> and MnO nanoparticles

Nabeen K. Shresta  
Physic self organized TiO<sub>2</sub> nanotubes. Formation, properties and applications

Angel Rubio  
Excited state properties of BN nanotubes optical and energy loss spectroscopies

Wolfgang Tremel  
Synthetic Approaches to Functionalized Chalcogenide Nanotubes

Daniel Kohler  
Double-walled bismuth-nanotubes from a chemical top-down – bottom-up approach

Jose I. Martinez  
Stability and electronic properties of TiO<sub>2</sub> nanostructures with and whituouth B and N doping,

Francesco Mercuri  
Polymorphism at the nanoscale and electronic properties of inorganic nanotubes:  
A theoretical approach

Mark Wilson  
The growth and structure of inorganic nanotubes

Sampsa Riikonen  
Computational study of BNNT catalytic synthesis

Dominik Eder  
Nanoengineering with residual Catalyst from CNT templates

David Tománek  
Studying local properties of MoxSylz nanostructures:From stability to electronic and vibrational structure

Gothard Seifert  
The Influence of Defects in Inorganic Nanotubes on Electronic and Mechanical Properties

Andrey Enyashin  
Structure and stability of Aluminosilicate Nanotubes

Agnieszka Kuc  
Shielding Nanotubes and wires with Imogolite: A route to create nanocables

Hegoi Manzano  
Structure and stability in Nanotubes of Cementitious Materials

Number of participants: 30

## Atom by Atom: NANO2009–Perspectives in nanoscience and nanotechnology

September 28-30, 2009

### CHAIRMEN

Pedro M. Echenique (DIPC and CSIC-UPV/EHU, Spain)

Jose M. Pitarke (CIC nanoGUNE, Spain)

### ORGANIZING COMMITTEE

Andreas Berger

Alexander Bittner

Rainer Hillenbrand

Luis Hueso

Igor Nabiev

Jose M. Pitarke

Daniel Sanchez-Portal

The "NANO2009 – Perspectives in Nanoscience and Nanotechnology" workshop is part of the Atom by Atom conference. NANO2009 followed the successful 'NANO2006 – Perspectives in Nanoscience and Nanotechnology' workshop celebrated in September of 2006 in Donostia-San Sebastian, Basque Country (Spain). It was a multidisciplinary workshop that reviewed the state of the art in the fields of nanomagnetism, nano-optics, self-assembly, nanobiotechnology, nanodevices, and theory and simulation at the nanoscale. NANO2009 fostered discussion on emerging applications with potentially significant impact for the materials, electronic, photonics, and life-science industries, and debate about the current strategy and perspectives in Nanoscience and Nanotechnology.

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### CONTRIBUTIONS

Emilio Artacho (Cambridge, UK)

Theoretical simulation of nanostructures: from oxide superlattices to topological defects in ferroelectric nanowires

Stephan Roche (Grenoble, France)

Mesoscopic transport in chemically modified forms of carbon based low-dimensional structures

Niek F. van Hulst (Barcelona, Spain)

Nanoscale control of single photon emitters by optical nano-antennas and tailored fs pulses

Stefan Maier (London, UK)

Coherent processes in plasmonic panocavities

Luis Martín-Moreno (Zaragoza, Spain)

Surface waves radiated by a subwavelength aperture in a metal film

2009

2009



Jean-Philippe Bourgoin (Gif-sur-Yvette, France)  
Issues related to self-assembly in the context of nanoelectronics

Christina Wege (Stuttgart, Germany)  
Nanoshaping with natural precision: self-assembled plant-viral templates as a novel scaffold toolkit

Alexander Govorov (Ohio, USA)  
Energy transfer in bio-inspired nanostructures

Stefan Haacke (Strasbourg, France)  
Ultrafast bio-molecular dynamics at the nanoscale

Sebastian Mackowski (Torun, Poland)  
Controlling absorption of light-harvesting complexes via plasmonic interactions

Gernot Güntherodt (Aachen, Germany)  
Spin currents in nanostructures

C. Leighton (Minnesota, USA)  
Magnetic phase separation at complex oxide interfaces

Josep Nogués (Barcelona, Spain)  
Exchange bias and proximity effects in  
'inverted' antiferromagnetic/ferrimagnetic core/shell nanoparticles

Klaus Ensslin (Zurich, Switzerland)  
Electrons in nanostructures — one by one

George Malliaras (Saint Etienne, France)  
Organic bioelectronics

Number of participants: 711

## BNC Tubes STREP Meeting

October 5-6, 2009

ORGANIZER  
Sampsa Riikonen (TKK, Finland)

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### CONTRIBUTIONS

#### Theoretical Studies on BNC Nanotubes and Their Synthesis

S. Riikonen

BN bond Stabilization on Iron and Magnesium

G. Lanzani

CN, CC and NN association reactions on a small nanosized cluster

L. Henrard

STM and Electronic Transport Fingerprints of B- and N-Doped Nanotubes

#### Synthesis of BNC Nanotubes

R. Fleurier

Sorting by density gradient ultracentrifugation of nanotubes

J. Lagoute

Measure of the electronic structure of SWNTs by STM

A. Nasibulin

Mechanistic Investigations of Single-Walled CNT Growth

T. Susi

N-doped SWCNT tube synthesis

J. Beausoleil

Synthesis of MWNT Doped with Nitrogen by FB-CVD

#### Characterization of BNC Nanotubes

E. Obratsova

Optical and low-field electron emission applications of nanotubes

A. Chernov

Separation on metallic and semiconducting fractions and characterization of single-wall carbon nanotubes

A. Koos

BNC tubes: synthesis and applications

Number of participants: 16

2009

2009

# Jülich Centre for Neutron Science Workshop 2009

## Trends and Perspectives in Neutron Scattering on Soft Matter

October 5-8, 2009

This international workshop was organized to discuss current status and future trends and possibilities of neutron scattering methods in studying structure and dynamics of soft matter systems. Due to the unique properties of neutrons investigations to reveal structure and dynamics of polymers, colloids, polymer interfaces, composite polymer materials, bio-compatible and bio-mimetic structures, polymer glasses and polymer nanostructures have delivered significant insight into soft matter physics and soft matter molecular structure. Novel dedicated methods as neutron spin echo spectroscopy or time resolved small angle neutron scattering have delivered unique insight into the understanding of soft matter structures and molecules. Recent advancements and future trends in soft matter science and their demands on neutron instrumentation were discussed.

2009

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### CONTRIBUTIONS

#### Slow Dynamics

Arantxa Arbe (UPV/EHU, Spain)

Nano-confinement through self-assembly in homopolymers with long alkyl sidegroups:  
Observation of anomalous relaxation

Christina Alba Simonesco (LLB Saclay, France)

Molecular weight dependence of the viscous slowing down and the glass properties of polymers

Michael Monkenbusch (Forschungszentrum Jülich, Germany)

Neutron Spin-Echo in Soft Matter and Biology, results from and challenges for the instrumentation

Jeremy C. Smith (Oak Ridge National Laboratory, USA)

Dynamics of Biomolecules

Hideki Seto (High Energy Accelerator Research Organization, Japan)

Multi-lamellar structure induced by hydrophilic and hydrophobic ions in a mixture of water and organic solvent

Thomas Hellweg (University of Bayreuth, Germany)

Responsive Microgels in the Presence of Different Counterions: The Hofmeister Effect

#### Kinetics

Reidar Lund (DIPC, Spain)

Fast Kinetic Processes in Micellar Systems Resolved by Small Angle Scattering

Stefan Egelhaaf (University of Düsseldorf, Germany)

Kinetics of structural transitions in surfactant solutions

Wim Pyckhout-Hintzen (FZ Jülich, Germany)

Molecular Rheology and Quenched Small Angle Scattering in Non-Linear Deformation

#### Instrumentation

Satoshi Koizumi (Japan Atomic Energy Research Institute, Japan)

Advanced Technique of Ultra-Small-Angle Neutron Scattering Explores a  
New Scientific Field of Neutron Cell Biology, Covering from a Single Molecule to Cell

#### Self Assembly

Mitsuhiro Shibayama (University of Tokyo, Japan)

Kinetics, structure, and dynamics of multi-arm poly(ethylene glycol) gels

Thomas Sottmann (University of Cologne, Germany)

Self-assembly in mixtures of water and super-critical CO<sub>2</sub>

Tim Salditt (Universität Göttingen, Germany)

Structure and Dynamics of Lipid Membranes by Inelastic Neutron Scattering and X-ray Imaging

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#### Nano Composites

Jean-Marc Zanotti (LLB Saclay, France)

Polymer dynamics under quasi-uniaxial confinement. The case of PEO in porous alumina

João Cabral (Imperial College London, United Kingdom)

Phase transitions in polymer-nanoparticle composites

Peter Schurtenberger (University of Fribourg, Switzerland)

Analyzing self-assembled protein clusters, gels and glasses using SANS and  
neutron spin-echo experiments

#### Synergies by Combination of Techniques

Peter Müller-Buschbaum (Technische Universität München, Germany)

Lateral structures at buried interfaces as probed with GISANS

Tiberio Ezquerro (CSIC-IEM, Spain)

Probing Ordering Processes in Soft Condensed Matter by using Time Resolved  
Techniques: from Neutrons to Photons

Michael Haertlein (Institut Laue Langevin, France)

Deuterium labeling of biological macromolecules at the ILL-EMBL Deuteration  
Laboratory, a platform of the Partnership for Structural Biology (PSB) Programme and  
its importance for Neutron Scattering studies in biology

Tom McLeish (Durham University, United Kingdom)

Neutron Flow-Mapping and Multiscale Modelling of Controlled-Architecture Polymer Melts

Number of participants: 22

## nanolCT School 2009 NanoPhotonics NanoOptics Modelling

October 26-30, 2009

### ORGANIZERS

Dr. Antonio Correia (Fundación Phantoms, Spain)  
Dr. Daniel Sanchez Portal (CSIC-UPV/EHU, DIPC, Spain)  
Dr. Igor Campillo (CIC nanoGUNE, NanoBasque, Spain)

Nanoelectronics represent a strategic technology considering the wide range of possible applications. Many of the potential emerging nanoelectronic 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 molecular and 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 emerging nanoelectronics 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. The EU funded nanolCT project (nº 216165) will establish a broad array of specialised training activities to provide mainly students with interdisciplinary competences in Nanotechnology and more specifically "nano-scale ICT devices & systems" (Emerging Nanoelectronics). These initiatives will generate a new generation of high-skilled interdisciplinary scientists, indispensable to the sustainability of European excellence in the topic considered, but also educate the current working force. The main training event will be a one post-graduate winter school on "ICT nanoscale devices" research domains organized in collaboration with the Donostia International Physics Center (DIPC), CSIC and nanoGUNE.

### CONTRIBUTIONS

#### School 1: NanoOptics and NanoPhotonics

Rainer Hillenbrand (CIC nanoGUNE, Spain)  
Juan Jose Saenz (UAM, Spain)  
Remi Carminati (ESPCI, France)

#### nanolCT symposium

Javier Aizpurua (CSIC-UPV/EHU, DIPC, Spain)

#### School 2: nanolCT modeling issues

Uzi Landman (Georgia Tech, USA)  
Stephan Roche (CEA-INAC, France)  
Javier Aizpurua (DIPC, Spain)  
Daniel Sanchez-Portal (CSIC-UPV/EHU, DIPC, Spain)

Number of participants: 127

## 5th Laser Ceramics Symposium: International Symposium on Transparent Ceramics for Photonic Applications

December 9-11, 2009

### ORGANIZING COMMITTEE

#### Chairman

J. Fernandez (UPV/EHU, Spain)

#### Co-chairs and Promoters

A.A. Kaminskii (Institute of Crystallography, Russian Academy of Sciences, Russia)

K. Ueda (Institute for Laser Science, University of Electro-Communications, Japan)

W. Strek (Institute of Low Temperature and Structure Research, Poland Academy of Sciences, Poland)

5th Laser Ceramics Symposium (LCS): International Symposium on Transparent Ceramics for Photonic Applications is a successive one just after the previous editions in Poland (2005), Japan (2006), France (2007), and China (2008). The aim of this Symposium is to provide a forum for material scientists, chemists and physicists to debate about the state of the art and the perspectives of nanocrystalline ceramics for photonic applications. It would also give to the participants an insight on future advances and research possibilities in these fields and an opportunity for starting fruitful collaborations. The following topics were explored:

Synthesis of optical transparent ceramics

Oxide and non-oxide laser ceramics

Characterization of physical properties

Optical spectroscopy

Composite structure

Ceramic lasers and amplifiers

Ultrashort pulse generation

Applications of optical ceramics

Novel materials and novel fabrication methods

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T. Taira (Laser Research Center for Molecular Science, Institute for Molecular Science, Japan)

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M. Mortier (Ecole Nationale Supérieure de Chimie de Paris, France)

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Number of participants: 55

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