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## 1st Baskrete Industry Open Days

March 13-14, 2012

### ORGANIZERS

Andrés Ayuela (DIPC, Spain)

Jorge S. Dolado (Tecnalia, Spain)

We presented our research in the field of nanoscience and nanotechnology for cementitious materials to local and international cement companies. The speakers provided practical insights to their research and discussion with industry offered trends for better applied research.

### CONTRIBUTIONS

**Welcome to DIPC** (Pedro M Echenique and Ricardo Díez Muiño, DIPC)

The nanoBasque Strategy: a vision of the future (Agencia nanoBasque-SPRI)

The nanoKER project (Jose M Pitarke, CIC nanoGUNE)

The Baskrete network (Jorge S Dolado, Tecnalia)

### Hydration of Clinker

Reactive Force Field Molecular Dynamics to Simulate the Hydration of Calcium Silicate Minerals

(Hegoi Manzano, UPV/EHU)

Atomistic simulations of anisotropic etching (Miguel Ángel Gosálvez, DIPC)

### Formation and Growth: C-S-H gel & crystalline phases

Monte-Carlo models of cement setting (Raquel González-Teresa, Tecnalia)

DFT simulations of Ettringite (Andrés Ayuela, DIPC)

### Nano – Confined Water

Nano-confined water (Silvina Cervený, CFM)

Challenges and progress in the atomistic simulation of liquid water

and wet interfaces (Emilio Artacho, CIC nanoGUNE)

### Industrial Experiences

Research & Development at Lafarge (Ellis Gartner, Lafarge)

Rheometry as a tool for investigating the Microstructure of Cement-based materials

(Maurizio Belloto, Bozzetto Group)

### Performance & Characterization

<sup>29</sup>Si NMR spectroscopy on cements: A theoretical study on CSH gel (Pawel Rejmak, DIPC)

Calcium leaching: A computational description (Juan José Gaitero, Tecnalia)

### Non-Portland Cements

The C-A-S-H gel of the Alkali Activated Cements (Jorge S. Dolado, Tecnalia)

### Organic - Inorganic Interactions

A first atomistic attempt... (Hegoi Manzano, UPV/EHU)

The soft hardening of cements (Jorge S. Dolado, Tecnalia)

### Nano-Additions and Nano - Reinforcements

Can cementitious nanotubes exist? (Andrés Ayuela, DIPC)

Self-healing cement-based materials (Edurne Erkizia, Tecnalia)

## Andreev Bound States and More

July 4-6, 2012

### ORGANIZERS

Sebastian Bergeret (Centro de Física de Materiales CSIC-UPV/EHU, Spain)

Cristian Urbina (CEA, Saclay, France)

This workshop brought together a group of leading scientists actively working on the detection and modeling of Andreev Bound States in superconducting nanostructures.

### CONTRIBUTIONS

Caglar Girit (CEA, Saclay, France)

Microwave spectroscopy of Andreev states in atomic contacts

Yuli Nazarov (University of Delft, Netherlands)

Singlet-Triplet manipulation of Andreev states in break junctions

Landry Bretheau (CEA, Saclay, France)

Modeling of spectroscopy of an atomic SQUID using a Josephson on-chip detector

Vitaly Shumeiko (Chalmers, Göteborg, Sweden)

Relaxation processes in Andreev levels system

Manuel Houzet (CEA, Grenoble, France)

Spin-boson description of the Andreev levels microwave spectroscopy experiments

Marcelo Goffman (CEA, Saclay, France)

Andreev Bound States and Kondo effect in carbon nanotubes

Alfredo Levy Yeyati (Universidad Autonoma de Madrid, Spain)

Interaction effects in Andreev and Majorana bound states in quantum dots

Guillermo Romero (UPV/EHU, Bilbao, Spain)

Circuit Quantum Electrodynamics with a Superconducting Quantum Point Contact

Andrew Doherty (University of Sydney, Australia)

A master equation approach to P(E) theory for the dynamical Coulomb blockade

Juan Carlos Cuevas (Universidad Autonoma de Madrid, Spain)

Microwave-assisted supercurrents and ac response of superconducting nanostructures

Fabio Pistolesi (University of Bordeaux, France)

Detection of ultrafast mechanical oscillations by exploiting Andreev bound states in superconducting junctions

Alvise Verso (DIPC, Spain)

Josephson current through a spin-filter

Philippe Joyez (CEA, Saclay, France)

Andreev Bound States and Kondo effect in carbon nanotubes

Hugues Pothier (CEA, Saclay, France)

Modeling of spectroscopy of an atomic SQUID using a Josephson on-chip detector

## NFO12 The 12th International Conference on Near-field Optics, Nanophotonics and related techniques

September 3-7, 2012

### ORGANIZERS

Javier Aizpurua (DIPC and CSIC-UPV/EHU, Spain)  
Rainer Hillenbrand (CIC nanoGUNE and Ikerbasque, Spain)

We celebrated the 20th anniversary of the international conference of Near-field Optics, Nanophotonics and Related Techniques (NFO) since its first edition in 1992. NFO has been among the first conferences addressing optics on the nanometer scale, triggered by the fascinating prospects of near-field techniques for pushing the resolution of optical microscopy towards the molecular level. Twenty years later, a variety of novel fields that involve nanooptics and photonics have been developed, including plasmonics, metamaterials, quantum information, biosensing and ultrafast dynamics. NFO12 covered all these fields, providing an international platform to present and discuss the latest advancements.



### CONTRIBUTIONS

Martin Aeschlimann (University of Kaiserslautern, Germany)  
Ultrafast optical control at the nanoscale

Dimitry N Basov (UC, San Diego, USA)  
Dirac plasmons in graphene: spectroscopy and imaging

Philip E Batson (Rutgers, The State University of New Jersey, USA)  
Plasmonic Forces Induced by Swift Electrons in Small Particles

Jeremy Baumberg (University of Cambridge, United Kingdom)  
Quantum Plasmonics in gap plasmons with precise sub-nm control

Oliver Benson (Humboldt University, Berlin, Germany)  
Fundamental Photonic Hybrid Systems Based on Defect Centers in Diamond

Richard Berndt (University of Kiel, Germany)  
Coupled plasmons at the transition from tunnelling to contact

Alexandre Bouhelier (Université de Bourgogne, Dijon, France)  
X(2) processes in electrically contacted optical gap antennas: second harmonic generation and optical rectification

Yannick De Wilde (CNRS, ESPCI, Paris, France)  
NSOM applications to plasmonics at infrared wavelength

Enzo Di Fabrizio (Istituto Italiano di Tecnologia, Genoa, Italy)  
Nanostructures and their use in nano optics

ZhenChao Dong (University of Science and Technology of China, Hefei, China)  
Plasmon mediated single molecular optoelectronics

Jens Dorfmueller (University of Stuttgart, Germany)  
Real-Space Imaging of Optical Nanoantennas by apertureless SNOM

Wolfgang Fritzsche (IPHT Jena, Germany)  
Biosensing at the single particle level

Javier García De Abajo (Institute of Optics, Madrid, Spain)  
Graphene plasmonics: An atomically thin look into NFO

Francisco García-Vidal (Universidad Autónoma de Madrid, Spain)  
Localized spoof surface plasmons in textured particles

Harald Giessen (Universität Stuttgart, Germany)  
Complex plasmonic nanostructures: moving towards applications

Haewook Han (Postech, South Korea)  
Quantitative Spectroscopic Terahertz Near-Field Microscopes

Achim Hartschuh (LMU Munich, Germany)  
New directions in tip-enhanced near-field optical microscopy

Christiane Hoepfner (University of Münster, Germany)  
Single Sphere and Self-similar Colloidal Nanoparticle Antennas for Membrane Protein Imaging

Mikael Käll (Chalmers University, Sweden)  
Nanoplasmonic biosensing – promises and problem

Femius Koenderink Amolf (Netherlands)  
Near-field measurement and manipulation of antenna-enhanced spontaneous emission

Frank Koppens (ICFO, Barcelona, Spain)  
Graphene plasmonics

Joachim Krenn (University of Graz, Austria)  
Tuning plasmon modes for biosensing

Kristján Leosson (University of Iceland)  
New fabrication approaches in low-loss plasmonics and controlled self-assembly of metal nanostructures for biosensing

Mikhail Lukin (Harvard University, Massachusetts, USA)  
Nanophotonics meets quantum optics

Adnen Mlayah Cemes (Toulouse, France)  
Acousto-Plasmonics based sensing

Hrvoje Petek (University of Pittsburgh, Pennsylvania, USA)  
Ultrafast plasmonics: Imaging light with electrons on the femto-nano scale

Albert Polman Amolf, Netherlands)  
Angle-resolved cathodoluminescence imaging Spectroscopy:  
deep subwavelength imaging of the modal dispersion of light

Anne Marie Pucci (Universität Heidelberg, Germany)  
Surface enhanced infrared spectroscopy

Romain Quidant (ICFO, Barcelona, Spain)  
Towards an integrated plasmonic platform for early cancer diagnosis

Mark Stockman (Georgia State University, Atlanta, USA)  
Spasing and Amplification in Plasmonic Nanosystems

Yung Doug Suh (Korea Research Institute Of Chemical Technology, Republic of Korea)  
Nano-gap Enhanced Raman Scattering (NERS) controlled by DNA

Prabhat Verma (Osaka University, Japan)  
High-resolution optical imaging through plasmonics and beyond plasmonics

Hong Wei (Chinese Academy of Sciences, Beijing, China)  
Controlling Surface Plasmon Modulations in Silver Nanowire Waveguides

Kumar Wickramasinghe (UC Irvine, California, USA)  
Raman Probe Force Microscopy – a New Method to Detect the Raman Effect

Jörg Wrachtrup (Universität Stuttgart, Germany)  
Near field imaging with single atomic emitters

Joel Yang (Institute of Materials Research and Engineering, Singapore)  
Driving Resonances In Plasmonic Nanoantennas By Electrons and Photons

## Superconducting Nanohybrids 2012

September 3-7, 2012

### ORGANIZERS

Sebastian Bergeret (Material Physics Center, CFM, Spain)  
Alexander Golubov (University of Twente, Netherlands)  
Andrei Zaikin (Karlsruhe Institute of Technology, Germany)

This workshop brought together leading scientists actively working in different sub-fields of mesoscopic superconductivity in order to discuss recent advances and overview the present status of the field, to visualize further research prospects and to promote new collaborations. The program will include talks by leading experts, both theorists and experimentalists, in topics such as: Unconventional pairing in superconductor-ferromagnet proximity structures, Proximity and Josephson effects in carbon nanotubes, graphene and topological insulator, Superconducting quantum dots, Quantum phase slips in superconducting nanowires and nanorings, Crossed Andreev reflection in NS and FS structures, Novel superconductors, Spintronics and superconductivity, Superconductivity and thermoeffects



### CONTRIBUTIONS

Teunis Martien Klapwijk (TU Delft, Netherlands)  
The evolution of superconducting hybrids

Leonid S Kuzmin (Chalmers University of Technology, Sweden)  
2D Arrays of Cold-Electron Bolometers for High- Performance Cosmology Experiments

Perti Hakonen (Aalto University, Helsinki, Finland)  
Hybrid Circuit Cavity Quantum Electrodynamics with a Micromechanical Resonator

Mikhail S. Kalenkov (Lebedev Physical Institute, Russian Academy of Sciences, Moscow, Russia)  
Giant thermoeffect in superconductors with magnetic impurities

Matthias Eschrig (Royal Holloway University of London, United Kingdom)  
Giant Nonlocal Thermoelectric Effects in Three-terminal Superconducting Devices

Francesco Giazotto (Scuola Normale Superiore-CNR, Pisa, Italy)  
Realizing heat interferometry through the Josephson effect

Pauli Virtanen (University of Würzburg, Germany)  
Absorption of heat into a superconductor —normal metal—  
superconductor junction from the electromagnetic environment

Clemens Winkelmann (Neel Institute, France)  
Electronic refrigeration and thermal couplings in superconducting hybrid devices

Konstantin Yu Arutyunov (University of Jyväskylä, Finland)  
Quantum phase slip junction

Oleg Astafiev (NEC Research Laboratories, Tsukuba, Japan)  
Coherent quantum phase slips in superconducting nano-wires

Frank Hekking (University Joseph Fourier, Grenoble, France)  
Quantum phase-slips in Josephson junction rings

Carmine Attanasio (University of Salerno, Italy)  
Quantum phase slips in superconducting Nb nanowire networks deposited on  
self-assembled Si templates

Evgeni Il'ichev (Jena, Germany)  
Dressed state amplification by a superconducting qubit

Julia Meyer (CEA-Grenoble, France)  
Andreev current induced by ferromagnetic resonance

Andrei Semenov (Lebedev Physics Institute, Moscow, Russia)  
Subgap electron transport in superconducting hybrids and Cooper pairs dephasing by  
electron-electron interactions

Venkat Chandrasekhar (Northwestern University, USA)  
Nonlocal correlations in a proximity-coupled normal metal

Tero Heikkilä (Aalto University, Finland)  
Manifestly non-Gaussian temperature fluctuations in superconductor-normal metal-superconductor structures

François Lefloch (CEA-Grenoble, France)  
Transport properties of diffusive three terminal hybrid superconducting S-N-S-N-S nanostructures

Jan Aarts (Leiden University, Netherlands)  
Aarts Long-ranged supercurrents in ferromagnetic CrO<sub>2</sub>

Victor Petrashov (Royal Holloway Un.of London, United Kingdom)  
Superconducting phase coherent electron transport in nano-engineered ferromagnetic vortices

Shiro Kawabata (National Institute of Advanced Industrial Science and Technology, Japan)  
A robust odd-frequency pairing in ferromagnet/superconductor junctions

Norman Birge (Michigan State University, USA)  
Spin-triplet supercurrent in ferromagnetic Josephson junctions

Mark Blamire (Cambridge University, United Kingdom)  
Spin currents in superconductors

Alvise Verso (Donostia International Physics Center, Spain)  
Spin-polarized Josephson and quasiparticle currents in superconducting spin-filter tunnel junctions

Alexander Brinkman (University of Twente, Netherlands)  
Josephson supercurrent through a topological insulator surface state

Manuel Houzet (CEA- Grenoble, France)  
Topological Josephson junctions out of equilibrium

Yasuhiro Asano (Hokkaido University, Japan)  
Majorana Fermions and Odd-frequency Cooper Pairs

Alexander Buzdin (University of Bordeaux, France)  
Vanishing Meissner effect as a hallmark of in-plane FFLO instability in  
superconductor-ferromagnet layered Systems

Avradeep Pal (University of Cambridge, United Kingdom)  
Spin filter tunnel junctions with superconducting electrodes Mohammad Alidoust:  
Unusual current-phase relation and magnetic interference pattern in non-aligned Josephson junctions

J Samuel Jiang (Argonne, USA)  
Unconventional proximity effect in ferromagnet/superconductor heterostructures with  
controlled magnetic non- collinearity

Jason Robinson (University of Cambridge, United Kingdom)  
Supercurrent enhancement in Bloch-like domain walls

Lenar Tagirov (Kazan University, Russia)  
Experimental Observation of the Triplet Spin-Valve Effect in a Superconductor-Ferromagnet Heterostructure

Anna Suszka (nanoGune, San Sebastian, Spain)  
Complex response of superconductivity to inhomogeneous magnetization states in  
epitaxial Nb/[DyFe<sub>2</sub>/YFe<sub>2</sub>]<sub>23</sub> multilayer

Yakov Fominov (Landau Institute, Russia)  
Odd-frequency-diamagnetic vs. odd-frequency- paramagnetic superconductivity

Valerii Vinokur (Argonne National Laboratory, USA)  
Magnetic field induced superconductivity in nanostructures

Mario Cuoco (CNR-SPIN, Italy)  
Odd-Frequency Triplet Pairing in Mixed-Parity Superconductors and in the presence of Rashba interaction

Audrey Cottet (CNRS Paris, France)  
Inducing triplet superconducting correlations in a normal metal wire

Detlef Beckmann (Karlsruhe Institute of Technology)  
Long-range spin transport in superconductors

Jukka Pekola (Aalto University, Finland)  
Statistics Of Dissipation In Superconducting Tunneling

Valery Ryazanov (Institute of Solid State Physics, Russia)  
Double proximity effect in hybrid planar Superconductor-(Normal metal/Ferromagnet)-Superconductor structures

Charis Quay Huei Li (Université Paris-Sud, France)  
Spin Imbalance and Spin-Charge Separation in a Mesoscopic Superconductor

Edward Goldobin (Tübingen University, Germany)  
Josephson junctions with magnetic field tunable current-phase relation

## JCNS and DIPC Joint Workshop: Trends and Perspectives in Neutron Scattering for Soft Matter and Biophysics

October 8-11, 2012

### ORGANIZERS

Dieter Richter (Jülich Centre for Neutron Science, Germany)

Juan Colmenero (Centro de Física de Materiales CSIC-UPV/EHU and DIPC, San Sebastián, Spain)

Neutron scattering has proven to be a key method to get deep insight into soft matter physics, biophysics and soft matter molecular structures. A comprehensive set of techniques is used to reveal the structure and dynamics of polymers, colloids, polymer interfaces, polymer composites and glasses as well as biomolecules, biocompatible and bio-mimetic structures. The aim of the international workshop jointly organized by the Jülich Centre for Neutron Science and the Donostia International Physics Center is to discuss the current status and the future trends and challenges of neutron scattering in this field. The workshop will bring experts together to address the following topics: Advanced Instrumentation for Soft Matter Research, Physics of Life, Kinetic Processes, Soft Materials for Energy Devices, Sustainable Polymers, Functional Materials, Synergies between Neutrons and Simulation, Nanostructured Systems

### CONTRIBUTIONS

Luigi Paduano (University of Naples "Federico II", Italy)

Nanodevices for antineoplastic diagnosis or therapy

Michael Gradzielski (Technische Universität Berlin, Germany)

Structure and dynamics of polyelectrolyte/surfactant complexes probed by SANS and NSE and their relation to the rheological properties

Mitsuhiro Shibayama (The University of Tokyo, Chiba, Japan)

Structure and gelation dynamics of tetra-PEG ion gels

Volker Urban (Oak Ridge National Laboratory, Tennessee, USA)

Neutron scattering for energy and the environment – light harvesting biofuels

Satoshi Koizumi (Ibaraki University, Hitachi, Japan)

In-situ observation of operating polymer electrolyte fuel cells (PEFC) by neutron small angle scattering – contrast variation by using deuterium gas

Regine von Klitzing (Technische Universität Berlin, Germany)

Stimuli sensitive polymer coatings with different film architectures

Stephan Förster (Universität Bayreuth, Germany)

Structure of soft lyotropic crystals and quasicrystals

Matthias Ballauff (Helmholtz Zentrum Berlin, Germany)

Small-angle neutron scattering – recent results on colloids and future trends

Sanat Kumar (Columbia University, New York, USA)

Modeling polymer nanocomposite structure and dynamics

Alessandro Paciaroni (University of Perugia, Italy)

Elastic and quasielastic neutron scattering investigation of biomolecules in glassy environments

Ralf Biehl (Forschungszentrum Jülich, Germany)

Proteins in solution: determination of domain structure and dynamics

Maikel Rheinstädter (McMaster University, Hamilton, Canada)

Frontiers in membrane biophysics

Victoria Garcia Sakai (ISIS, Didcot, United Kingdom)

Views from a soft matter neutron instrument scientist

Bernhard Frick (Institut Laue Langevin, Grenoble, France)

New developments in neutron backscattering with applications in soft matter and perspectives for studies of slow dynamics

Juan Colmenero (Centro de Física de Materiales CSIC-UPV/EHU and DIPC, San Sebastián, Spain)

Chain dynamics in un-entangled polymer blends with dynamic asymmetry.

A generalized Rouse incoherent scattering function based on the GLE formalism

Isabelle Grillo (Institut Laue Langevin, Grenoble, France)

Recent applications of time resolved SANS combined with a stopped-flow equipment

Toshiji Kanaya (Kyoto University, Japan)

Flow-induced polymer crystallization – effects of molecular weight and shish-kebab formation

## Surface Dynamics: Beyond the Born-Oppenheimer Static Surface Approximation

October 24-26, 2012 | Universidad de Zaragoza, Spain

### ORGANIZERS

Cristina Díaz (Universidad Autónoma de Madrid, Spain)

Manuel Alcamí (Universidad Autónoma de Madrid, Spain)

Sergio Díaz-Tendero (Universidad Autónoma de Madrid, Spain)

Maite Alducin (CSIC-UPV Materials Physics Center and DIPC, San Sebastián, Spain)

Roar A. Olsen (SINTEF Materials and Chemistry, Oslo, Norway)

To present, most of the study performed on molecule/surface interactions have taken advantage of the Born-Oppenheimer static surface (BOSS) approximation. To unravel the role played by non-adiabatic effects on these systems represents a new challenge for surface science physicists. Evidence of non-adiabatic effects has been found, for example, for metal with low work functions through chemi-currents measurements. But, the main question to be answered now is relative to the role that electron hole pair excitations could play in reactive and non-reactive scattering of molecules, both open-shell and close-shell ones, with metal surfaces, and to the role played by phonon excitations.

The scope of this workshop has been to serve as meeting point for theoretical and experimental scientists working on the field, which allows them to identify problems of interest for experimentalists, to identify bottlenecks on actual theoretical methods, and to exchange new ideas that could be used to overcome some of the actual shortcomings. This objective has been fully fulfilled, thanks to the good balance between theoretical and experimental talks at the workshop. The experimentalists have pointed out the need to go beyond the Born-Oppenheimer static surface (BOSS) approximation in order to properly describe, for example, phenomena relative to femtochemistry. The workshop has also allowed to establish the state-of-the-art of the development on nonadiabatic dynamical methods.

### CONTRIBUTIONS

Rainer Beck (Ecole Polytechnique fédérale de Lausanne, Switzerland)

State-resolved gas/surface reactivity measurements: evidence for mode- and bond selective chemisorption of methane on Ni and Pt

Eckart Hasselbrink (Universität Duisburg-Essen, Germany)

Non-Adiabaticity in Surface Chemical Reactions Studied Using Thin Metal Film Heterostructures

Alberto Pablo Sánchez Muzas (Universidad Autónoma de Madrid, Spain)

Vibrational deexcitation and rotational excitation of H<sub>2</sub> and D<sub>2</sub> scattered from Cu(111): adiabatic versus non-adiabatic dynamics

Paul Tiwald (Vienna University of Technology, Austria)

Charge exchange between a proton and a lithium fluoride surface: an embedded cluster approach

Fernando Martín (Universidad Autónoma de Madrid, Spain)

Commensurate solid-solid phase transitions in self-assembled monolayers of alkythiolates lying on metal surfaces

Alec Wodtke (Max Planck Institute for Biophysical Chemistry, Germany)

Surface Dynamics: Beyond the Born-Oppenheimer Static Surface Approximation

Daniel Auerbach (University of California, USA)

on-adiabatic electronic effects in energy transfer at metal surfaces: do we need to go beyond electronic friction models?

Iñaki Juaristi (UPV/EHU, Spain)

Role of energy loss channels in the reactive and non-reactive dynamics of molecules and atoms on metal surfaces

Peter Kratzer (University Duisburg-Essen, Germany)

Energy dissipation at surfaces by anharmonic vibrational coupling and electron-hole pair excitation

Pascal Larregaray (ISM, UMR5255, CNRS/U.Bordeaux1, France)

Dynamical reaction pathways in Eley-Rideal recombination of Nitrogen from W(100)

Francesco Nattino (Leiden Institute of Chemistry (LIC), Leiden University, Netherlands)

Ab-Initio Molecular Dynamics study of CHD<sub>3</sub> dissociation on Pt(111): the role of the v<sub>1</sub>-normal mode pre-excitation

Remi Petuya (ISM, UMR5255, CNRS/U.Bordeaux1, France)

Theoretical analysis of the dynamics of N<sub>2</sub> scattering on W(100) surface

Maitreyi Robledo Relaño (Universidad Autónoma de Madrid, Spain)

Charge transfer in molecules and ultrathin insulating films deposited on metal surfaces

Phillip Thomas (Leiden University, Netherlands)

Sum-of-Products Representation of Potential Energy Surfaces using the Chebyshev n-mode Approach: Application to 6D Gas-Surface Reactive Scattering Problems

Martin Wolf (Fritz Haber Institute, Berlin, Germany)

From surface femtochemistry to ultrafast phase transitions in CDW systems

Peter Saalfrank (Institut für Chemie, Universität Postdam, Postdam-Golm, Germany)

Vibration-phonon and vibration-electron hole pair coupling at surfaces

Maria Blanco-Rey (DIPC, Spain)

Vibrational excitation of hydrogen atoms in palladium by ballistic electrons

Rachel Crespo-Otero (Max-Planck-Institut für Kohlenforschung, Germany)

Photochemistry of N-Methylformamide: Matrix Isolation and Nonadiabatic Dynamics

Jean-Pierre Gauyacq (Université de Paris-Sud, France)

Magnetic (spin) transitions in adsorbates at surfaces induced by tunnelling electrons

Thomas Frederiksen (DIPC, Spain)

Theory and simulation of vibrational spectroscopy and adsorbate dynamics with inelastic tunneling electrons

Thorsten Kluener (University of Oldenburg, Germany)

Ab-initio surface photochemistry

Myrta Grüning (University of Coimbra, Portugal)

Ab-initio many-body perturbation-theory: overview and perspectives

Geert-Jan Kroes (Leiden Institute of Chemistry, Leiden University, Netherlands)

Quantum and Ab Initio Molecular Dynamics calculations on scattering of H atoms and H<sub>2</sub> molecules from metal surfaces

Daniel Fariás (Universidad Autónoma de Madrid, Spain)

Molecular beam studies of the dissociation of H<sub>2</sub> and O<sub>2</sub> on metal surfaces

Mark Wijzenbroek (Leiden Institute of Chemistry, Leiden University, Netherlands)

Static surface temperature effects on the dissociation of H<sub>2</sub> and D<sub>2</sub> on Cu(111)

Joerg Meyer (Technische Universität München, Germany)

Better than the BOSS: Watching phonons cool down during oxygen dissociation on Pd(100)

## Controlled Atomic Dynamics on Solid Surfaces: Atom and Molecular Manipulation

May 13-16, 2013

### ORGANIZERS

Thomas Frederiksen (DIPC, San Sebastián, Spain)

Nicolás Lorente (CIN2, Barcelona, Spain)

Magnus Paulsson (Linnaeus University, Sweden)

The objective of this workshop was to provide a thorough picture of the existing theoretical techniques and how they are contributing to the understanding and quantitative prediction of controlled manipulations. Equivalently, the workshop aims at exposing present experimental developments and challenges that need to be addressed by new theoretical developments. The meeting will steer discussions and collaborations much needed to add momentum to a developing field. This workshop can be of landmark importance since no equivalent workshop or conference has been organized with the aim of making "controlled manipulations" a full-fledged research field.

This workshop was dedicated to Prof. Hiromu Ueba and to all of his contributions to this field.

### CONTRIBUTIONS

Maite Alducin (CFM-CSIC, San Sebastián, Spain)

Does N<sub>2</sub> adsorption increase on strained Fe monolayers?

Richard Berndt (Kiel University, Germany)

Manipulation of the spin and charge states of adsorbed molecules

María Blanco-Rey (DIPC, San Sebastián, Spain)

Subsurface Hydrogen and Deuterium Manipulation by Ballistic Electrons

Marie-Laure Bocquet (ENS Lyon, France)

Understanding Inelastic Electron Spectroscopy of single adsorbates on metal surfaces:

start «small», finish «big»

Mads Brandbyge (DTU Nanotech, Denmark)

Electron-Phonon coupling and molecular dynamics in the presence of current

Eugene Chulkov (CSIC-UPV/EHU, Spain)

Relativistic effects in surface electronic structure of solids: Bychkov-Rashba systems and topological insulators

Karl-Heinz Ernst (EMPA, Switzerland)

Chirality in molecular recognition and dynamics at surfaces

Aran Garcia-Lekue (DIPC, San Sebastián, Spain)

Azobenzene-Based Single-Molecule Junctions: Charge Transport Mechanism and IETS Fingerprints



Michael Galperin (UC San Diego, USA)  
Molecular junctions: A nonequilibrium atomic limit

Jean-Pierre Gauyacq (CNRS Paris-Sud, France)  
Excitation of magnetic adsorbates by tunnelling electrons: atoms and chains

Axel Gross (Ulm University, Germany)  
Molecule-surface interactions at complex metal-gas and metal-liquid interfaces studied by ab initio molecular dynamics simulations

Werner Hofer (Liverpool University, UK)  
Theory of scanning tunneling microscopy: studying dynamic processes

Maki Kawai (RIKEN, Tokyo, Japan)  
Local Symmetry Rules Spin Ground State: FePc on Au(111)

Tadahiro Komeda (Tohoku University, Japan)  
Manipulation of Spin in Double Decker Phthalocyanine Molecule

Rolf Möller (Duisburg-Essen University, Germany)  
Revealing molecular dynamics through scanning noise microscopy and spectroscopy

Karina Morgenstern (Ruhr-Universität Bochum, Germany)  
Inelastic spectroscopy with sub-atomic resolution

Hiroshi Okuyama (Kyoto University, Japan)  
Controlled switching molecule-electrode interfaces

Richard Palmer (Birmingham University, UK)  
Atomic manipulation by electron injection

Jose-Ignacio Pascual (CIC nanoGUNE, San Sebastián, Spain)  
Spin, Forces and Photons in Molecular Tunneling Junctions

Bo Persson (Forschungszentrum Jülich, Germany)  
Charging and Bond formation of Adsorbates on Ultrathin, Insulating Films Supported by a Metal Substrate

Mats Persson (Liverpool University, UK)  
Tribology at the atomistic level

Hrvoje Petek (Pittsburgh University, USA)  
A multi-state single-molecule switch actuated by rotation of an encapsulated cluster within a fullerene cage

Roberto Robles (CIN2, Spain)  
Site- and orbital-dependent charge and spin manipulation in supported transition metal phthalocyanines

Ruslan Temirov (Forschungszentrum Jülich, Germany)  
Imaging and control of large organic molecules within a scanning probe microscopy junction

Sergei Tikhodeev (GPI Moscow, Russia)  
Mechanisms of rotation of a single acetylene molecule on Cu(001) by tunneling electrons in STM

Tchavdar Todorov (Queens University Belfast, UK)  
Interatomic forces under current

Hiromu Ueba (Toyama University, Japan)  
Vibrationally mediated single molecule reactions in real space and in real time

Martin Wolf (Fritz-Haber MPG, Berlin, Germany)  
Probing the transient electronic structure in surface femtochemistry

## 2nd Baskrete Industry Open Days

May 28-29, 2013

### ORGANIZERS

Andrés Ayuela (DIPC, Spain)  
Jorge S. Dolado (Tecnalia, Spain)

The Baskrete initiative is a collaborative project within the Campus of International Excellence Euskampus carried out between the Basque University (UPV/EHU), the Materials Physics Center (MPC), the Donostia International Physics Center (DIPC) and Tecnalia with a twofold mission: On the one hand, BASKRETE will coordinate all the actions which are currently underway in the Basque Country in the field of nanoscience and nanotechnology for cementitious materials. On the other hand, Baskrete aims to trigger the transfer of high technology knowledge to companies through the establishment of a cooperative program with the industrial agents.

The Baskrete Open Days target to industrials but it will be relevant to anyone (in academia, national research institutes or industry) with experience/expertise in cementitious materials and anyone interested in the latest achievements and about the short and long term prospects in this promising field.

Baskrete acknowledges the funding received from NANO-IKER project (IE11-304), within the Eortek program of the Department of Industry, Innovation Trade and Tourism of the Basque Government.



### CONTRIBUTIONS

P.M. Echenique and R. Díez Muiño (DIPC)  
Welcome to DIPC

A. Martínez Muro (nanoBasque)  
EHS Advance, safety nanotechnologies for companies

J. Campas (Euskampus)  
Euskampus: community of Knowledge poles

J.S. Dolado (Tecnalia)  
The Baskrete initiative

S. Shah (Northwestern University, USA)  
Nanomodification of cementitious materials with nanoparticles

H. Manzano (UPV/EHU)  
Hydration of clinker phases using molecular simulations

A. Ayuela (DIPC)  
Structure, atomistic simulations and phase transitions of stoichiometric yeelimite

J.S. Dolado (Tecnalia)  
Early growth of C-S-H gel

J.J. Gaitero (Tecnalia)  
Aging and durability of ternary cements containing fly ash and activated paper sludge

M. Belloto (Bozzetto Group)  
Superfluid pumpable concrete:  
the role of superplasticizers on performances, robustness and chesiveness

P. Rejmak (DIPC)  
29Si chemical shift anisotropies in hydrated calcium silicates: a computational study

H. Manzano (UPV/EHU)  
Sheer deformations in the C-S-H gel: understanding the moleclar mechanism of creep

J.S. Dolado (Tecnalia)  
Multi-scale modeling of cement-based materials: structure performance linkage

A. Ayuela (DIPC)  
Do cementitious nanotubes exist?

## 30th Brandt Ritchie Workshop (BRW)

October 1-4, 2013

### ORGANIZERS

Andres Arnau (CFM CSIC-UPV/EHU and DIPC, Spain)  
Joseba Iñaki Juaristi (CFM CSIC-UPV/EHU and DIPC, Spain)  
Pedro Miguel Echenique (DIPC and CFM CSIC-UPV/EHU, Spain)

### COMMITTEE

Néstor Arista (Centro Atómico Bariloche, Argentina)  
Amand Lucas (University of Namur, Belgium)  
Raúl Baragiola (University of Virginia, USA)  
R.H. Ritchie (ORNL, USA)  
Salvador Cruz (UNAM, Mexico)  
John R. Sabin (University of Florida, USA)  
Pedro Miguel Echenique (DIPC, Spain)  
Helmut Winter (Humboldt University, Germany)  
Vladimir Esaulov (ISMO, France)  
Jorge Valdés (USM, Valparaíso, Chile)  
Fernando Flores (UAM, Spain)  
Yasunori Yamazaki (RIKEN, Japan)

The topics within BRW cover various fields of condensed matter physics or material science. In particular, the following subjects were addressed: Particle-solid interactions with special attention to charge exchange, energy loss and related phenomena; collective excitations in low-dimensional systems; induced excitation of surface and bulk plasmon states; dynamic charge states in ion-solid interactions; electron dynamics in nanostructures; photonic and transport properties of materials; radiation interaction with organic and inorganic nano-materials; related processes at surfaces, interfaces and nanostructures. Following the spirit of previous Brandt Ritchie Workshops, participants presented recent results of their research activity.

This edition paid homage to Rufus Ritchie, an outstanding physicist, who has realized seminal contributions to the fields of atomic physics and interaction of atoms with matter. Prof. Rufus Ritchie was given an honorary degree from the University of the Basque Country.

The BRW workshop took place at Donostia International Physics Center (Donostia-San Sebastián).

### CONTRIBUTIONS

Peter Bauer (JKU Linz, Austria)  
Electronic stopping of slow light ions in metals and insulators

Aitor Bergara (UPV/EHU, Spain)  
Emergence of new low-energy plasmons under pressure

María S. Gravielle (Instituto De Astronomía y Física del Espacio (IAFE), Argentina)  
Grazing incidence fast atom diffraction from metal surfaces

Natalia E. Koval (Centro De Física De Materiales and Consejo Superior de Investigaciones Científicas, Spain)  
Energy loss and charge transfer processes during photoemission from metal clusters and adsorbates

Sir John B. Pendry (Imperial College London, United Kingdom)  
Challenges in Surface Plasmonics

Fernando Flores (Universidad Autónoma de Madrid, Spain)  
Inelastic tunneling spectroscopy for magnetic atoms and the Kondo resonance

Archie Howie (University of Cambridge, United Kingdom)  
Thermal Fluctuations and Decoherence in Electron Microscopy

Christoph Lemell (Vienna University of Technology, Austria)  
Classical simulations for surface-streaking experiments

Karoly Tokesi (MTA Atomki, Hungary)  
Can the ions be guided with MeV/amu energies? The case of 1 MeV proton microbeam

Vito Despoja (University of Zagreb, Croatia)  
Electron loss and photoemission spectra in pristine and doped graphene

Jorge Esteban Miraglia (Instituto de Astronomía y Física del Espacio, Argentina)  
Electron impact multiple ionization

Raúl Antonio BARAGIOLA (University of Virginia, USA)  
Electron emission by rare gas ions on Cs coated Al surfaces

Julio Ferrón (Intec Conicet Unl, Argentina)  
Unoccupied band states and ion induced electron emission

Juana Gervasoni (Cnea-Conicet, Argentina)  
Plasmon excitations in single-walled carbon nanotubes by impact of charged particles

María Luz Martiarena (Conicet, Argentina)  
Li<sup>+</sup> neutralization on nanostructures of Au: size effects on the charge exchange process

Nerea Zabala (UPV/EHU, Spain)

Electromagnetic interaction between relativistic electrons and bounded targets

Amand Lucas (University of Namur, Belgium)

Giant phonon tsunami caused by energetic ions skipping on a polar surface

Andrés Ayuela (Donostia International Physics Center, Spain)

Computational  $^{29}\text{Si}$  NMR in Hydrated Portland Cement

Richard A. Wilhelm (Helmholtz-Zentrum Dresden – Rossendorf,

Institute of Ion Beam Physics and Materials Research, Germany)

Interaction of Slow Highly Charged Ions with Free-Standing 1nm Thick Carbon Nano-membranes

Maia G. Vergnori (Donostia International Physics Center, Spain)

Exchange interaction and its tuning in magnetic binary chalcogenides

Aran García-Lekue (Donostia International Physics Center, Spain)

Intermolecular H-Bonding for Porphyrin Molecules on Surfaces

María Blanco Rey (Donostia International Physics Center, Spain)

Efficient Eley-Rideal reactions with large projectiles made possible:

$\text{N}_2$  formation by pick-up of N-adsorbates off Ag(111)

John R. Sabin (University of Florida, USA)

Coupled Cluster Calculation of Atomic Mean Excitation Energies

Salvador Cruz-Jimenez (Universidad Autónoma Metropolitana, Mexico)

Study of Many-electron Atom Confinement by Padded Open and Closed Boundaries

Remigio Cabrera-Trujillo (Instituto de Ciencias Físicas, Unam, Mexico)

Universal scaling behavior for the electronic stopping cross section of protons on atomic and molecular targets

Moni Behar (Universidade Federal Do Rio Grande Do Sul, Brazil)

Coulomb heating behavior of fast light diclusters through the Si<110> direction:

influence of the mean charge state

Edith Goldberg (Intec Unl Conicet, Argentina)

How do surface energy gaps and image states affect the neutralization of  $\text{Li}^+$  in the scattering by metal surfaces?

Laura Isabel Fernández (Donostia International Physics Center, Spain)

Co nanodot arrays grown on a ferromagnetic GdAu<sub>2</sub> template:

substrate/nanodot antiferromagnetic exchange coupling

Vyacheslav Silkin (Donostia International Physics Center, Spain)

Acoustic plasmons in extrinsic free-standing graphene

Rosa Monreal (Universidad Autónoma de Madrid, Spain)

Quantum Plasmonics?

Helmut Winter (Humboldt University, Germany)

Recent progress in Fast Atom Diffraction

Rubén Esteban Llorente (Donostia International Physics Center, Spain)

Effect of quantum tunneling in plasmonics: theory and experiments

Andreas Heidenrich (UPV/EHU, Spain)

Coulomb explosion of doped helium clusters

Eduardo C. Montenegro (Ufrj, Rio de Janeiro, Brazil)

Electron loss and energy loss

Jaume Navarro (Department of Logic and Philosophy of Science (UPV/EHU) and Ikerbasque, Spain)

Niels Bohr in Manchester. A hundred years of the quantum atom

