

Seminars

09/01/2015

Water and water/metal interfaces from first principles.

Prof. Marivi Fernandez-Serra

Stony Brook University, New York, USA

13/01/2015

Detection of multipartite entanglement close to symmetric Dicke states.

Prof. Geza Giedke

Max-Planck-Institut für Quantenoptik, Garching, Germany

13/01/2015

Magnetic response of functionalized lipid bilayers.

Dr. Joachim Kohlbrecher

Paul Scherrer Institut, Villigen, Switzerland

14/01/2015

Hamiltonian adaptive QM/MM: multi-scale modeling of chemical reactions in solution.

Prof. Rosa Bulo

University of Utrecht, The Netherlands

15/01/2015

Direct growth of 2D materials on practical substrates: from surface chemistry to new physics and devices.

Prof. Jeffrey A. Kelber

University of North Texas, Denton, USA

29/01/2015

latrochemistry, cannabis and drug design.

Prof. Pilar Goya Laza

Instituto de Química Médica (CSIC), Madrid, Spain

30/01/2015

Landscape without neutrinos.

Prof. Juan José Gómez-Cadenas

Instituto de Física Corpuscular CSIC-UV, Valencia, Spain

06/02/2015

Interactions between layers in ferroelectric superlattices.

Prof. Matthew Dawber

Stony Brook University, New York, USA

10/02/2015

Detecting quantum entanglement in multiparticle systems.

Dr. Geza Toth

Ikerbasque, Department of Theoretical Physics, UPV/EHU, Leioa, Spain

12/02/2015

Hunting for helical boundary states and Majoranas in superconductor-topological insulator-superconductor hybrid junctions.

Prof. Arturo Tagliacozzo

Università di Napoli Federico II, Napoli, Italy

13/02/2015

Quantum optics without photons from basic effects to new quantum information architectures.

Martin Schütz (PhD student)

MPQ Garching, Germany

16/02/2015

Contributions of Physics to Ethics: Nuclear Weapons, Free Will, and the Good Life.

Prof. Carl Mitcham

Colorado School of Mines, USA

16/02/2015

Electrical and thermal control of magnetic exchange interactions.

Prof. Jonas Fransson

Uppsala University, Sweden

18/02/2015

Chemical bonding in the light of an energy decomposition analysis.

Prof. Gernot Frenking

Fachbereich Chemie, Philipps Universität Marburg, Marburg, Germany

24/02/2015

Attosecond time-resolved photoemission experiments in cross comparison to spin resolved photoemission spectroscopy.

Prof. Ulrich Heinzmann

University of Bielefeld, Molecular & Surface Physics Bielefeld Institute for BioPhysics &

NanoScience (BINAS) Bielefeld, Germany

25/02/2015

Attosecond electron dynamics in complex molecular systems.

Dr. Andrea Trabattoni

Politecnico di Milano, Milano, Italy

26/02/2015

Development of the PETAL laser facility and its applications in physics.

Prof. Dimitri Batani

Université de Bordeaux, Talence, France

27/02/2015

Rare earth doped fluoride materials for optics and photonics.

Prof. Michel Mortier

ParisTech, Ecole Nationale Supérieure de Chimie de Paris, France

06/03/2015

Scanning tunneling spectroscopy of the superconducting vortex lattice.

Dr. Isabel Guillamon Gomez

Instituto de Ciencia de Materiales Nicolás Cabrera, Condensed Matter Physics Center,

Universidad Autónoma de Madrid, Spain

09/03/2015

Nanostructured graphene: challenges in fabrication and modeling.

Prof. Antti-Pekka Jauho

Center for Nanostructured Graphene (CNG), DTU Nanotech,

Technical University of Denmark, Lyngby, Denmark

10/03/2015

Towards a chemically accurate description of reactive molecule-surface scattering.

Prof. Geert-Jan Kroes

Leiden Institute of Chemistry, Gorlaeus Laboratory, Leiden, The Netherlands

16/03/2015

Graphene-metal interaction revealed by scanning tunneling microscopy.

Dr. Hyowon Kim

Samsung Advanced Institute of Technology (SAIT) Yeoungtong-gu, Suwon-si, Korea

18/03/2015

La divulgación científica. Un cuento inexacto.

Dr. Ana Montserrat Rosell

TVE programa Tres14, Madrid, Spain

20/03/2015

Density functional theory based strategies for patterning and etching of semiconductor surfaces.

Dr. Sananda Biswas

International Centre for Theoretical Physics (ICTP), Trieste, Italy

25/03/2015

Step polymerization in various solvent conditions.
A computer simulation approach using "Patchy Brownian Cluster Dynamics".
Dr. Jean-Christophe Gimel
Micro and Nano-medicine Laboratory, University Hospital in Angers, France

26/03/2015

Linear and nonlinear surface polaritons in graphene-based structures.
Prof. Yuliy Bludov
Center for Physics, University of Minho, Braga, Portugal

15/04/2015

Plasmons in nanographene and other atomic scale systems
Prof. Javier García de Abajo
ICFO-The Institute of Photonic Sciences, Castelldefels, Barcelona, Spain

24/04/2015

Strong field atomic ionization with linear and circular polarized light:
Spectra, cusps and time delay.
Prof. Anatoli Kheifets
Australian National University, Canberra, Australia

28/04/2015

ARPES insight into the dual nature of f- electrons in rare-earth intermetallics.
Prof. Denis Vyalikh
Dresden University of Technology, Dresden, Germany

29/04/2015

Exploring matter under extremes conditions at the linac coherent light source.
Eduardo Granados
SLAC National Accelerator Laboratory, Stanford University, California, USA

04/05/2015

Electronic and vibrational properties of TiSe_2 in the charge-density wave phase from first principles.
Dr. Raffaello Bianco
Paris VI (UPMC), France

08/05/2015

Beyond the Born-Oppenheimer approximation in matter under extreme conditions.
Prof. J. Alfredo Caro
Los Alamos National Laboratory, New Mexico, USA

19/05/2015

Basics and applications of nonlinear dielectric techniques.
Prof. Ranko Richert
Arizona State University, Tempe, USA

21/05/2015

Bound states in the continuum in graphene based nanostructure.
Prof. Luis Rosales Ahumada
Universidad Técnica Federico Santa María, Chile

22/05/2015

Outlook in neutrino physics.
Prof. Pilar Hernández Gamazo
Instituto de Física Corpuscular CSIC-UV, Valencia, Spain

29/05/2015

Quantum Engineering with ultracold matter.
Dr. Omjyoti Dutta
Jagiellonian University, Krakow, Poland

02/06/2015

Engineering of the electronic and opto-electronic properties of carbon nanotubes
via artificially induced defects and electrostatic doping.
Dr. Gilles Buchs
Swiss Center for Electronics and Microtechnology, CSEM, Switzerland

03/06/2015

Current topics in attosecond photoemission spectroscopy on metal surfaces and interfaces.
Dr. Martin Schäffer
Technische Universität München (TUM), Germany

05/06/2015

Charge transfer between donor-acceptor molecular networks on metal surfaces.
Dr. Jonathan Rodriguez Fernandez
IMDEA, Madrid, Spain

18/06/2015

Chemical Structures and mechanical properties of molecules studied by high-resolution force microscopy.
Dr. Shigeki Kawai
University of Basel Switzerland PRESTO and Japan Science and Technology Agency, Kawaguchi, Japan

24/06/2015

Dopants acting as trap for electrons: Spin relaxation and decoherence.
Prof. María Chamarro Calvo
Pierre and Marie Curie University, Institut des NanoSciences de Paris, France

24/06/2015

Modelling colloidal semiconductor nanocrystals: towards realistic sizes.
Dr. Ivan Infante
Vrije Universiteit Amsterdam, The Netherlands

26/06/2015

**k-resolved electronic structure by soft-X-ray ARPES:
From 3D systems to buried interfaces and impurities.**

Dr. Vladimir N. Stokov

Swiss Light Source and Paul Scherrer Institute, Villigen-PSI, Switzerland

26/06/2015

Vibronic structure methods: from small molecules to systems with hundreds of atoms.

Prof. Robert Berger

Philipps-Universität Marburg, Germany

02/07/2015

Robust electron pairing in the integer quantum hall effect regime.

Prof. Moty Heiblum

Weizmann Institute of Science, Rehovot, Israel

06/07/2015

Simple design of topological state.

Dr. Xiao Hu

International Center for Materials Nanoarchitectonics (WPI-MANA)

National Institute for Materials Science (NIMS)

Tsukuba, Japan

21/07/2015

Quantum Optics in waveguides.

Prof. Luis Martín Moreno

Instituto de Ciencia de Materiales de Aragón, (ICMA), Zaragoza, Spain

22/07/2015

One electron reduced density matrix of strong correlation harmonium atom.

Dr. Jerzy Cioslowski

University of Szczecin, Poland

24/07/2015

Electrical contacts to two-dimensional materials: when less is more.

Dr. Xavier Cartoixa Soler

Universidad Autónoma de Barcelona, Spain

30/07/2015

STM-based spectroscopies of single-molecule and single-atom contacts.

Richard Berndt

Institute of Experimental and Applied Physics, University of Kiel, Germany

04/08/2015

Manipulation of the induced pair potential in topological insulator-superconductor hybrid junctions.

Dr. Pablo Burset Atienza

University of Würzburg, Germany

07/08/2015

Mesoscopic and nonequilibrium superconductivity in nano hybrids.

Prof. Teunis Klapwijk

Delft University of Technology, The Netherlands

11/09/2015

Many-body interaction induced exotic phenomena at surface: molecular Kondo effect and inelastic process in laser-photoemission.

Prof. Emi Minamitani

Graduate School of Engineering

The University of Tokyo, Bunkyo-ku, Tokyo, Japan

18/09/2015

Novel 2D electron gases at the surface of transition-metal oxides.

Prof. Andres Felipe Santander Syro

CSNSM, Université Paris-Sud, France

22/09/2015

CO₂ capture in aqueous solutions: insights from ab initio simulations.

Prof. Wanda Andreoni

Ecole Polytechnique Federale de Lausanne, EPFL Institute of Theoretical Physics, Lausanne, Switzerland

30/09/2015

Understanding the stiffness of Macromolecules: From single chains to semi flexible polymer brushes.

Prof. Kurt Binder

Johannes Gutenberg University, Mainz, Germany

06/10/2015

La labor de la Fundación Española para la Ciencia y la Tecnología: participación social en la ciencia.

Prof. José Ignacio Fernandez Vera

FECYT, Madrid, Spain

09/10/2015

Atomic clocks and other marvels of absolute frequency measurements.

Prof. Amand Lucas

University of Namur, Belgium

21/10/2015

The role of short-range order and hyperuniformity in the formation of band gaps in 2D disordered photonic materials.

Dr. Luis Froufe Perez

University of Fribourg, Switzerland

22/10/2015

Single-atom optical clocks.

Prof. David Jeffery Wineland

NIST, Boulder, Colorado, USA

Workshops

29/10/2015

Image processing tools for the study of brain connections.

Dr. Ignacio Arganda Carreras (Ikerbasque Fellow)
University of the Basque Country, UPV/EHU, Spain

06/11/2015

Hybrid upconversion nanomaterials for photochemotherapy.

Luca Salassa
CIC BiomaGUNE, Donostia/San Sebastián, Spain

11/11/2015

Stellar occultations: Chariklo and its ring system.

Rodrigo Leiva
Instituto de Astrofísica, Facultad de Física, Pontificia Universidad Católica de Chile.
Observatoire de Paris, LESIA, France

19/11/2015

Topologically confined states at corrugations of gated bilayer graphene.

Dr. Marta Pelc
CFM, Centro de Física de Materiales, Donostia/San Sebastián, Spain

15/12/2015

100 años de Relatividad General.

Prof. Alberto Galindo Teixaire
Ex-Presidente de la Real Academia de Ciencias Exactas, Físicas y Naturales

Theory for Planar Molecular and Atomic Scale Devices

January 26-28, 2015

Donostia International Physics Center, Donostia/San Sebastián
http://dipc.ehu.es/ws_presentacion.php?id=116

Organizing Committee

Daniel Sánchez-Portal (CFM CSIC-UPV/EHU, DIPC)
Mads Engelund (CSIC, Madrid)
Thomas Frederiksen (DIPC, Ikerbasque)
Aran García-Lekue (DIPC, Ikerbasque)

The aim of the workshop was to bring together some of the groups working actively on the field (singularly those involved in the European Integrated Fp7 FET project PAMS, contract number 610446). The explored atomic and molecular devices included dangling bond circuitries, functionalized by coupling with organic molecules, and controlled by remote alteration of molecular states by local band bending. Multibranch polyaromatic logical gates addressed by nanowires were also explored.

The development of new methodological tools, allowing for a multiscale description (using from first-principles to empirical force-fields) of the structural, electronic and transport properties of such atomic and molecular devices was also discussed. The ultimate aim was to optimize the design and synthesis of atomic and molecular gates by developing these new theoretical tools.

Invited Speakers

Ville Loukonen, Hugo Pinto, Juha Ritala, John Tracey and Adam Foster (Aalto University)

Mads Engelund from (CSIC)

Thomas Frederiksen (Ikerbasque, DIPC)

Benoit Eydoux, Ghassen Dridi, Omid Faizy (CEMES-CNRS, Toulouse)

Andrii Kleshchonok, Thomas Lehmann (Dresden University of Technology)

Daniel Sánchez-Portal (CFM CSIC-UPV/EHU, DIPC)