

# VISITING RESEARCHERS

**DIPC understands that modern science entails the constant exchange of knowledge and experience to the benefit of all involved.**

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## LONG VISITS

### PROF. J. ALONSO

Universidad de Valladolid, Spain

01-09-2002 through 31-08-2003

During my Sabatical stay at DIPC, I have investigated on several topics in the general field of Nanostructures, in collaboration with DIPC and UPV scientists and students.

- Structural and chemical properties of carbon nanotubes: Absorption and storage of Hydrogen. Intercalation of alkali atoms in graphite and nanotubes. Computer simulation of the formation process and growth of nanocones.
- Electronic and chemical properties of atomic clusters: Optical properties. Interaction of metallic clusters with Hydrogen. Metastable states of multiply charged clusters. The dynamics of excited states in density functional theory, with applications to molecular dissociation and Coulomb explosion in nanostructures.
- Electronic correlations in atoms and clusters.

### DR. F. AUZEL

CNRS, UMR, Meudon, France

28-10-2003 through 30-01-2004

Powder coherent sources both of the superradiant (SR) and Amplified Spontaneous Emission (ASE) types [1,2,3,4].

### DR. A. BORISOV

Université Paris Sud, France

01-05 through 26-06-2003

“Building up the screening below the femtosecond scale”

Time dependent density functional theory is used to study short-time dynamics of the screening of charges suddenly introduced in a free electron gas. The electron gas is modeled with a finite-size jellium cluster. We find that the screening is built-up locally on a time scale well below the femtosecond for typical metallic densities. At this ultrashort time scale, the time evolution is not affected by the cluster boundary conditions, and our results apply to the infinite system as well. The results for different electronic densities can be understood in terms of universal scaling laws.

### PROF. A. GALINDO

Universidad Complutense Madrid, Spain

09-11 through 20-12-2003

Quantum information and quantum algorithms. Basic problems in Quantum Physics. Completion of a two-volume textbook on Advanced Quantum Mechanics, and a textbook on Space-Time Structure.

**PROF. B. GUMHALTER**

University of Zagreb, Croatia

01-11-2001 through 28-02-2002

Several topics have been planned to be studied and discussed with the researchers and Ph.D. students during the visit to the DIPC:

- Decoherence effects associated with spatio-temporal propagation of electron-hole pairs optically excited in the bands of image potential at metal surfaces.
- Assessment of the respective roles of plasmons and electron-hole pairs in two-dimensional surface bands in the screening properties of surfaces.
- Effects of electron-hole coupling on the lifetime of quasiparticles in the states of surface potential.
- Excitation of surface phonons or charge density fluctuations in scattering of atoms and molecules from metal surfaces.

**DR. W.A. HOFER**

University College London, U.K.

14-09 through 31-10-2002

First Principles Calculations of Electronic Structure of Solid Surfaces using the DFT code VASP, as well as obtaining STM images using his own code bSKAN. Since then, he is collaborating with Andres Arnau in a project to study inelastic tunneling currents in metallic contacts and another one to characterize the adsorption of Oxygen on Ruthenium (0001) surfaces.

**PROF. A. KAMINSKII**

Russian Academy of Sciences, Russia

02-10 through 31-12-2002

Professor Alexander A. Kaminskii is acknowledged leader in the basis research of the physics and spectroscopy insulating laser and nonlinear-laser crystals among the world solid-state laser community. He is being recognized for his fundamental contributions in Ln<sup>3+</sup>-doped crystals and characterization of their spectroscopic and physical properties. Present scientific interests are in the field of nonlinear-laser crystals and nanocrystalline ceramics.

**DR. A. KAZANSKIY**

University of St. Petersburg, Russia

01-10 through 30-11-2003

Electron dynamics at adsorbates on metals

**DR. Y. KOROTEEV**

Institute of Strength Physics and Materials Sciences, Tomsk, Russia

01-12-2001 through 28-02-2002, 06-07 through 06-10-2002 and

26-02 through 26-05-2003

First-principles calculations of the surface electronic structure of La(001) and Lu(0001).

First-principles film linear augmented plane wave calculations have been performed for La(0001) and Lu(0001). The d-surface states have been obtained at all symmetry points of the Brillanin zone. The dispersion of surface state at the  $\Gamma$  point was used for interpretation of the scanning-tunneling spectroscopy measurements of the lifetime broadening on both Lu(001) and La(0001).

**DR. G. LEMELL**

University of Technology, Vienna, Austria

07-01 through 11-02-2003

Many Electron Systems Interacting with Strong Field.

**DR. M. LÖFFLER**

Lehrstuhl für Festkörperphysik, Erlangen, Germany

02-04 through 30-09-2002

Co and Ag nanostructures on Si surfaces.

Vicinal surfaces with high density of steps are natural templates for the growth of regular arrays of dots, wires and stripes. In this project we have studied by means of Scanning Tunneling Microscopy the reactive deposition epitaxy of cobalt silicides on vicinal Si(111) substrates. Contrary to initial expectations, the growth process is simplified with respect to the flat surface. A single precursor species, i.e. the Co ring structure, leads to a rapid build up of silicide clusters, regularly spaced along the steps, although incoherently arranged across the terraces. Currently we are analyzing more quantitatively the different morphologies and stoichiometries observed as a function of coverage and deposition temperature.

**DR. J. MAHECHA**

Universidad de Antioquia, Medellin, Colombia

12-08 through 09-12-2002

Electron dynamics of atoms adsorbed in metallic surfaces

- Semi-classical propagation and spectral analysis in the negative Hydrogen ion interacting with a metallic surface: A semiclassical propagator method combined with harmonic inversion of short time signals is used to find the resonant states of an electron interacting with a H atom near a metallic surface. A semi classical propagator approach is used to calculate an approximation to the autocorrelation function entirely in terms of classical trajectories. A filter-diagonalization method for harmonic inversion of the complex time signal is applied to extract the resonances.

- Stabilization and complex scaling approaches to find resonant states of an electron interacting with an atomic core and a metallic surface are applied with similar purposes of those of (i) and using different models for the electron-surface interaction.

- The electron-core-surface system in the regime of large atom-surface distances is studied by using different methods. Initially a generalized van der Waals interaction model is used.

Tasks (i) and (ii) are developed with participation of two researchers of DIPIC and (iii) with participation of two researchers of La Rioja University. Two students and a researcher from UdeA are involved in the development of the project.

**PROF. I. NAGY**

Technical University Budapest, Hungary

03-09 through 26-10-2002, 05-05 through 27-06-2003 and

02-10 through 30-11-2003

Study based on a scattering approach of short-range correlations in an electron gas has been developed. In this work, the pair-correlation function at zero interparticle separation  $g(0)$  of an interacting electron gas is derived by an averaging procedure using the exact enhancement factor for scattered waves of electrons in a model potential. The range of

the screened potential is fixed by a physically motivated constraint. Agreement with the result of a many-body method based on summation of ladder diagrams for electron-electron interactions is established. As a possible application of the potential a nontrivial density-scaling in the thermal resistivity of metals is predicted.

**DR. V. POPOV**

Altai State Technical University, Barnaul, Russia  
18-05 through 14-08-2002 and 01-12-2002 through 28-02-2003  
Theory of excitations in small atom clusters.  
Ground states properties of small magnetic clusters of 3d-atoms.

**DR. G. ROUSSINA**

Russian Academy of Sciences, Tomsk, Russia  
03-04 through 14-06-2003  
Surface phonons in CuPd surface alloys.

**PROF. W. SCHATTKE**

Universität Kiel, Germany  
26-10 through 12-2002 and 01-12-2003 - 29-02-2004  
Photoemission from core and valence levels in gas-phase atoms, solids and surfaces: We have developed a generalization of the multiple scattering theory to treat non-spherical potentials. This allows us to make a more accurate description of the photoemission process, which is relevant for many new experiments. For example, during the past few years the experimental advances have permitted the measurement of the angular distributions of photoelectrons emitted from free molecules fixed in space. Previous to this work, free-molecule studies were limited to orientationally-averaged measurements, thus limiting the information derivable from the data. The dependence of such fixed-in-space angular distributions on photon energy provides an exciting new probe of electronic structure and dynamics. With our new method we can accurately calculate the angular distributions of photoelectrons emitted from core levels of small molecules with definite orientations in space. The results are found to be in excellent agreement with recent extensive sets of experimental data. The theory can also be applied to the study of other more complex problems as well, as for example in the study of low-energy photoemission and photoelectron diffraction processes from the valence band of low-symmetry systems (such as clusters and adsorbates), for which the application of standard one-step models is problematic.

**DR. I. SKLIADNEVA**

Russian Academy of Sciences, Tomsk, Russia  
05-04 through 30-06-2002  
Phonon spectra in bulk metals and at metal surfaces.  
Relaxation and phonon spectra of surface alloys of palladium on Cu(100) have been studied by using embedded atom method. The calculation showed complex character of the surface relaxation and very strong Pd-Cu interatomic interactions which explain the experimentally observed alloy surface phonon models. First-principles calculations have been done for phonon spectra of MgB<sub>2</sub> to compare them with the recently measured spectra of this material. Very high frequency models obtained can explain the importance of the phonon contribution to the lifetime broadening of electron states in MgB<sub>2</sub>.

**DR. T. STRASSER**

Universität Kiel, Germany  
03-08 through 29-11-2002

Photoelectron diffraction for electronic and structural characterization of solid crystal surfaces.

This visitor has used his expertise in calculating photoemission intensities from first principles in a one-step model approach to the case of aluminium (111) surfaces. His theory has permitted explaining recent experimental spectra that have resulted in the first accurate experimental determination of high-energy conduction bands in a solid surface. Part of his work during his stay at DIPC has been also devoted to the study of photoemission from stepped surfaces with full inclusion of multiple scattering. This part of his work is still underway.

**DR. T. TEPERIK**

Russian Academy of Sciences, Saratov, Russia  
02-11 through 22-12-2002

Optical response of metallic metamaterials

Description: The research of Dr. Teperik during his stay at San Sebastian was focused on understanding the behaviour of light in interaction with metallic metamaterials composed of subwavelength air inclusions in silver, gold, and other metals. Her calculations showed that the reflectivity from the surfaces of this type of materials exhibits strong reflection and transmission resonances that can be attributed either to localized Mie modes of the inclusions or to Bragg reflections in the case of ordered arrays of inclusions. This is an ongoing work, and actually, Dr. Teperik is now progressing in the understanding of these materials while she continues performing calculations from Saratov.

## SHORT VISITS

**DR. M. AESCHLIMANN**

Universität Essen, Germany

08-03 through 11-03-2003

Ultrafast two-photon photoemission studies of excited electrons in metals.

**PROF. M. AGUILA**

CIEMAT-CSIC, Spain

11-07 through 14-07-2002

Particle physics: current status and perspectives.

**DR. R. AGUADO**

ICMM-CSIC, Spain

09-05 through 09-05-2003

Kondo effect in quantum dots.

**PROF. F. AGULLÓ**

Universidad Autónoma de Madrid, Spain

04-09 through 06-09-2002

Ion beam techniques in the analysis of materials.

**DR. J. AIZPURUA**

National Institute of Standards and Technology (NIST), Gaithersburg, USA

05-09 through 05-09-2002

Tunnel-coupled quantum dots : Atomistic Theory of Quantum Dot Molecules and Arrays.

**PROF. P.M. AJAYAN**

Rensselaer Polytechnic Institute, New York, USA

12-06 through 15-06-2002

Synthesis, Mechanical and electronic properties of carbon nanotubes and their assemblies.

**PROF. G. ALEJALDRE LOSILLA**

CIEMAT, CSIC, Spain

28-02 through 28-02-2003

Fusion energy and the ITER project: present situation and future perspectives.

**PROF. J. ALONSO**

Universidad de Valladolid, Spain

10-05 through 13-05-2002

Hydrogen adsorption in carbon nanotubes.

**DR. F. ARYASETIAWAN**

Research Institute for Computational Science (RICS), Japan

13-01 through 20-01-2002

Total energy method from many-body formulation.

**PROF. M.C. ASENSIO**

C. LURE, France - ICMM-CSIC, Madrid, Spain

17-02 through 20-02-2002

Fermi Surface Mapping of 2-D and 3-D Systems by Angle Resolved Photoemission.

**PROF. DR. N.W. ASHCROFT**

Cornell University, Ithaca, New York, USA

26-03 through 17-04-2002 and 11-06 through 07-2003

Theory of Many Particle Systems, Density Functional Theory (Classical and Quantum), and Theory of Dense Hydrogen and Matter under Extreme Conditions.

**PROF. R. BARAGIOLA**

University of Virginia, Charlottesville, USA

01-04 through 03-04-2003

Electronic excitation of insulating materials by slow ions: overview and the MgO case.

**DR. N. BARBERÁN FALCÓN**

Universidad de Barcelona, Spain

26-10 through 28-10-2003

Nanostructures under magnetic fields.

**PROF. S. BARONI**

SISSA and INFN DEMOCRITOS National Simulation Center, Trieste, Italy

09-11 through 11-11-2003

Monte Carlo simulation of the dynamics of quantum interacting systems: Structure, dynamics, and superfluidity of small doped He clusters.

**DR. A. BAUER**

Freie Universität Berlin, Germany

20-02 through 25-02-2002

Electronic Structure and Lifetimes of Surface States on Lanthanide Metals.

**PROF. M.C. BELLISSENT-FUNEL**

CNRS, Laboratoire Leon Brillouin LLB, Saclay, France

09-01 through 12-01-2003

Protein dynamics studied by Neutron Scattering and Molecular Dynamics Simulations.

**PROF. G. BENEDEK**

Università degli Studi di Milano - Bicocca, Italy

22-11 through 26-11-2002

Surface phonons and phase transitions.

**PROF. G.F. BERTSCH**

Editor Review of Modern Physics

University of Washington, USA

01-11 through 10-11-2002

Optical response of nanostructures.

**DR. G. BIHLMAYER**

IFF-FZ, Forschungszentrum Jülich, Germany

17-05 through 23-05-2003

Magnetism in low dimensions: Overlayers, wires and atoms.

**PROF. J. BLANCO**

Universidad de Oviedo, Spain

05-06 through 06-06-2002

Neutron Scattering.



**PROF. S. BLÜGEL**

Forschungszentrum Jülich, Germany  
12-11 through 15-11-2002 and 14-12 through 18-12-2003  
**Magnetism at the Nanocosmos.**  
Rashba spin-orbit effect at metal surfaces.

**DR. M. BODE**

Universität Hamburg, Germany  
16-07 through 21-07-2003  
**Atomic resolution in magnetic STM.**

**PROF. D. BOERMA**

Universidad Autónoma de Madrid, Spain  
03-09 through 06-09-2002  
**Atomic Collisions in Solids. Surface Physics and Computer Simulations.**

**DR. A. BORISOV**

Université Paris Sud, France  
04-05 through 31-05-2002, 01-12 through 05-12-2002 and 22-11 through 29-11-2003  
**Time Dependent Density Functional Theory of screening in metallic clusters.**  
Building up the screening below the femtosecond scale.

**DR. I. BOUSTANI**

Universität Wuppertal, Germany  
15-08 through 15-09-2003  
**Boron quasiplanar clusters and nanotubes. From theoretical predictions to experimental confirmations.**

**J. BRAVO ABAD**

Universidad Autónoma Madrid, Spain  
09-10 through 10-10-2002  
**Superprism effect in photonic crystals.**

**PROF. L. BREY**

ICMM-CSIC, Spain  
23-01 through 24-01-2003  
**A lattice spin mechanism for colossal magnetoresistance in manganites.**

**DR. T. BRIXNER**

University of California, Berkeley, USA  
03-12 through 07-12-2003  
**Adaptive Quantum Control: Technique and Applications**

**DR. D. CANGIALOSI**

University of Delft, The Netherlands  
16-11 through 17-11-2003  
**Positron annihilation lifetime spectroscopy to study the dynamics of polycarbonate far below T<sub>g</sub>.**

**DR. M.A. CAZALILLA**

ICTP, Trieste, Italy  
09-01 through 12-01-2002, 04-06 through 06-06-2002, 09-07 through 12-07-2002 and 16-12 through 20-12-2002  
**Strongly correlated systems.**  
Some scenarios for strong correlation phenomena in ultracold atom systems.

**DR. S. CERVENY**

Chalmers University of Technology, Sweden  
07-12 through 15-12-2003

General framework of dynamic properties of glass forming polymers by dielectric spectroscopy in combination with other experimental techniques and MD-simulations.

**DR. A. CLIMENT FONT**

Universidad Autónoma de Madrid, Spain  
04-09 through 06-09-2002

Interaction of Energetic Ions with Solids, RBS and ERDA techniques.

**PROF. E. CORONADO MIRALLES**

Universidad de Valencia, Spain  
25-04 through 26-04-2002

Materiales Moleculares Multifuncionales.

**PROF. V. CRESPI**

University of Pennsylvania, USA  
30-05 through 02-06-2002

Electronical and mechanical properties of nanotubes.

**A. CHAUTY**

Université de Paris-Sud, France  
29-07 through 30-07-2002

Effect of the hydrostatic pressure on the dynamics of polymer materials.

**PROF. M. DÄHNE**

Technische Universität Berlin, Germany  
01-04 through 06-04-2002

Quantum dots and nanowires of rare-earth silicides studied with STM.

**PROF. P. DE ANDRES**

ICMM-CSIC, Spain  
21-11 through 22-11-2002

How do water molecules bind to close-packed metal surfaces?

**PROF. P. DEDERICHS**

Forschungszentrum Jülich, Germany  
09-11 through 15-11-2002

Diluted Magnetic Semiconductors.

**PROF. B. DELOCHE**

Université Paris-Sud, France  
07-05 through 09-05-2002, 19-02 through 23-02-2003, 13-07 through 15-07-2003 and  
27-08 through 29-08-2003

Dynamics of Polymers in confined geometries.

**DR. A. DERESZEWSKA**

Merchant Maritime University, Gdynia, Poland  
06-09 through 06-10-2002

Dielectric relaxation of semirigid polymers in polar solvents. (Phase Transitions in Liquid Crystalline Polymer Solutions by means of Dielectric Spectroscopy)

**DR. L. DESPONT**

Université de Neuchâtel, Switzerland

11-11 through 14-11-2003

Photoelectron diffraction: structural studies of surface reconstruction of ferroelectrics and implications on spontaneous polarization.

**DR. D. DICKERSCHIED**

Universiteit Utrecht, Holland

05-08 through 20-08-2003

Cold atoms bose-Einstein condensation in cold atoms systems and optical lattices.

**PROF. J. DOBSON**

Griffith University, Australia

14-09 through 28-09-2003

Van der Waals interactions at leisure.

**PROF. T.W. EBBESEN**

Université Louis Pasteur, Strasbourg, France

24-10 through 27-10-2002

Extraordinary transmission through subwavelength holes.

**PROF. T. FAUSTER**

Lehrstuhl für Festkörperphysik, Erlangen, Germany

21-07 through 24-07-2003

Inter- and intraband scattering by defects at metal surfaces.

**PROF. J. FINK**

Institute for Solid State Research. IFW. Dresden, Germany

27-11 through 01-12-2002

Plasmons in solids studied by electron energy-loss spectroscopy.

**DR. V. FRANCO PUNTES**

Universidad de Barcelona, Spain

18-03 through 21-03-2003

Nanoparticles: Building units and built structures.

**DR. L.S. FROUFE PÉREZ**

Universidad Autónoma de Madrid, Spain

01-06 through 08-06-2003

Conductance Distributions in Disordered Wires at the Metal-Insulator Crossover.

**PROF. A. GALINDO**

Universidad Complutense Madrid, Spain

30-09 through 01-10-2003

Quantum information and quantum algorithms. Basic problems in Quantum Physics. Completion of a two-volume textbook on Advanced Quantum Mechanics, and a textbook on Space-Time Structure.

**DR. A. GARCÍA ARRIBAS**

Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain

07-11 through 07-11-2003

Effective-Hamiltonian Simulations in Ferroelectrics

**PROF. F. GARCÍA MOLINER**

Universitat Jaume I, Castellón, Spain

02-10 through 04-10-2003

The practical value of culture.

**PROF. M.E. GARCÍA**

Frei Universität Berlin, Germany  
15-02 through 15-02-2002

Laser induced ultrafast phase transitions.

**PROF. J. GÓMEZ**

Universidad Autónoma de Madrid, Spain  
28-02 through 01-03-2002

Microscopía de proximidad: los ojos de la nanotecnología.

**PROF. J.C. GÓMEZ SAL**

Universidad de Cantabria, Spain  
05-06 through 06-06-2002

About non Fermi liquids and the cuantic phase of transitions in metals. An experimental approach.

**DR. M. GRÜNING**

Universiteit van Amsterdam, The Netherlands  
11-08 through 12-08-2003

Study of the role of exchange and correlation effects in both ground state density functional theory as well for excitation within time-dependent density-functional theory.

**PROF. F. GUINEA LÓPEZ**

ICMM-CSIC, Spain  
08-10 through 12-10-2003

Suppression of Quantum features and decay processes induced by metallic environments.

**PROF. B. HELLSING**

Chalmers and Göteborgs University, Sweden  
22-04 through 28-04-2002, 17-11 through 24-11-2002 and 01-07 through 31-07-2003

Electron-phonon interactions on metal surfaces.

The influence of the electron-phonon coupling on lifetimes of excited electron and hole states.

**PROF. A. HERNANDO**

Universidad Complutense de Madrid, Spain  
30-09 through 01-10-2002

Magnetism of nanocrystalline iron.

**PROF. F. HIMPSEL**

University of Wisconsin, Madison, USA  
11-07 through 18-07-2002

Au and Ag nanostructures and atom chains on Si surfaces.

**DR. A.F. HO**

University of Birmingham, U.K.  
01-03 through 30-03-2003

Effects of disorder in one-dimensional quantum liquids, and phase diagram of binary mixtures of one-dimensional harmonic fluids.

**DR. W.A. HOFER**

University of Liverpool, U.K.  
15-01 through 17-01-2003

Theory of scanning tunnelling microscopy.

**PROF. P. HOFMANN**

University of Aarhus, Denmark  
04-12 through 08-12-2002

Geometry, electronic structure and electron-phonon coupling on Bi surfaces.

**PROF. K. HORN**

Fritz-Haber- Institut Berlin, Germany  
04-05 through 07-05-2002

High resolution photoemission spectroscopy from nanostructures.

**PROF. I. HOWARD**

Universiteit Antwerpen, Belgium  
05-06 through 19-06-2003

Structural properties of small clusters with DFT techniques.

**PROF. A. HOWIE**

Cavendish Laboratory, Cambridge, U.K.  
10-09 through 24-09-2002, 04-07 through 12-07-2003 and 03-09 through 17-09-2003  
Physics of electron microscopy, including elastic and inelastic scattering of electrons, electron interference and electron energy loss spectroscopy, secondary electron emission and ionisation damage. Surface science, catalyst particles, crystal defects and solid state excitations.

Theory of valence electron excitations by fast electrons.

**PROF. S. IIJIMA**

Meijo University, Japan  
11-04 through 13-04-2002

Carbon nanostructures: nanotubes, onions, cones.

**DR. A. KAZANSKIY**

University of St. Petersburg, Russia  
14-05 through 15-05-2003

Electron dynamics at adsorbates on metals.

**DR. C. KOLLATH**

Lehrstuhl für Theoretische Festkörperphysik, München, Germany  
04-11 through 01-12-2003

Ultra cold atoms optical lattices non equilibrium phenomena and Bose-Fermi mixtures.

**PROF. E. KRASOVSKII**

Universität Kiel, Germany  
09-05 through 13-05-2002, 08-07 through 05-08-2002,  
27-11 through 02-12-2002 and 04-08 through 29-08-2003

First-principles calculations of collective excitations in bulk metals.

Electronic structure and dielectric properties of heavy metals: Bi, La, and Lu.

Dielectric properties and collective excitations in heavy metals.

**□. KRUPIN**

Free Universität Berlin, Germany  
13-01 through 25-01-2003

Structural and electronic studies using photoelectron diffraction from solid surfaces.

**DR. J. KUNTZE**

Universität Kiel, Germany  
22-09 through 29-09-2003

“One-dimensional atom chains”

We have started a new project focused on the structural properties of one-dimensional Au atom chains grown on Si(111) vicinal surfaces. Such atomic chains are potential candidates to exhibit one-dimensional Luttinger liquid behaviour. Previous experiments display exotic properties, like fractional band filling. Moreover, they are expected to undergo a structural charge-density wave transition at low temperature, which could be directly observed at our STM chamber.

**PROF. DR. V. KUZNETSOV**

Tomsk State University, Russia  
06-04 through 04-05-2002

Density functional methods in the theory of phase diagrams of alloys and in the Kondo effects.

**DR. N. LORENTE**

Université Paul Sabatier, Toulouse, France  
16-10 through 17-10-2002

Controlled reactions on single molecules on surfaces.

**PROF. E. LUDEÑA**

IVIC, Caracas, Venezuela & Universidad Autónoma de Madrid, Spain  
25-06 through 29-06-2003

Is DFT a semi-empirical theory? Some comments on its foundations, accomplishments and shortcomings.

**DR. R. MAGYAR**

Rutgers University, USA  
16-03 through 19-03-2003

Study of the role of exchange and correlation effects in both ground state density functional theory as well for excitation within time-dependent density-functional theory.

**PROF. N.H. MARCH**

Universiteit Antwerpen, Belgium  
01-11 through 30-11-2002 and 28-05 through 25-06-2003

Study of the role of exchange and correlation effects in both ground state density functional theory as well for excitation within time-dependent density-functional theory.  
Correlation functionals in DFT.

**PROF. M. MARESCHAL**

CECAM, ENS-Lyon, France  
29-04 through 29-04-2002

Statistical mechanics applied to granular materials and polymers.

**DR. C. MARINICA**

CNRS, Laboratoire des Collisions Atomiques et Moléculaires, Orsay, France  
22-01 through 25-01-2003

Electron excitations at metal surfaces covered with noble gas atoms.

**PROF. R. MATZDORF**

Universität Würzburg, Germany

23-10 through 28-10-2003

Electron correlations and electron-phonon coupling in adsorbates on noble-metal surfaces.

**PROF. F.J. MESEGUER**

Unidad Asociada CSIC - UPV, Física Aplicada, Spain

04-03 through 05-03-2002

Photonic crystals and related structures.

**PROF. J.E. MIRAGLIA**

IAFE and Universidad de Buenos Aires, Argentina

16-09 through 16-09-2003

Plasmon Decay and Nonlinear Effects.

**PROF. R. MIRANDA**

Universidad Autónoma de Madrid, Spain

26-05 through 27-05-2003

Tunnelling Spectroscopy on metallic nanostructures: observing the electronic states of confined systems.

**DR. P. MOLINÁS I MATA**

Universidad Politécnica de Catalunya, Spain

22-04 through 22-04-2003

“Two-dimensional diffusion of vacants on Ge(111) surfaces”

Atomic defects at Ge(111) surfaces display a rich, temperature diffusion behaviour. They act as single particles with isotropic or anisotropic diffusion, depending on temperature and vacant concentration. In this project we prepare highly perfect Ge surfaces and create vacants with the STM tip. The diffusion properties of such vacants will be studied as a function of temperature.

**PROF. G. MORATA**

Centro Biología Molecular - Universidad Autónoma Madrid, Spain

23-09 through 23-09-2002

Science and Society at the dawn of the XXI Century - Social Impact of Biological Techniques.

**PROF. R. MUKHOPADHYAY**

Solid State Physics Division, BARC, India

10-11 through 13-11-2003

Stochastic Dynamics in Condensed Matter: Neutron Scattering Study.

**PROF. I. NAGY**

Technical University Budapest, Hungary

03-01 through 01-02-2002

Spin effects in electron lifetimes.

**PROF. V. NAZAROV**

Kyushu Institute of Technology, Kitakyushu, Japan

11-07 through 10-08-2002 and 09-02 through 07-03-2003

Bulk and surfaces plasmons.

Collective excitations in bulk metals and at their surfaces.

**DR. M. NEEB**

BESSY Cmbh, Berlin, Germany

19-02 through 23-02-2003

Ultrafast relaxation dynamics of optically excited states in small transition metal clusters.

**DR. P. ORDEJÓN**

ICMAB-CSIC, Spain

08-04 through 12-04-2003

First principles calculations of ballistic transport in nanoscale systems.

**DR. J. ORTEGA MATEO**

Universidad Autónoma de Madrid, Spain

08-11 through 09-11-2002

Dynamical fluctuations and the  $\sqrt{3}\times\sqrt{3}$  transition in  $\alpha$ -Sn/Ge(111) and Sn/Si(111).**DR. R. OTERO**

STM de Miranda, Madrid, Spain

18-02 through 01-03-2002

Ag-Au stripes and lateral superlattices.

**DR. J.J. PALACIOS**

Universidad de Alicante, Spain

21-03 through 22-03-2002

Molecular electronics from first principles.

**DR. I. PASCUAL**

ICMAB-CSIC, Spain

19-12 through 22-12-2002

STM in lateral nanostructures.

**PROF. J. PENDRY**

Imperial College London, U.K.

12-05 through 16-05-2003

The Perfect Lens - Focusing Beyond the Diffraction Limit.

**PROF. J. PERDEW**

University of Tulane, New Orleans, USA

13-07 through 19-07-2003

Climbing Jacob's Ladder: The Meta-Generalized Gradient Approximation for Exchange and Correlation.

**DR. W. PFEIFFER**

Universität Würzburg, Germany

18-09 through 22-09-2002

Electron Dynamics in Supported Nanoparticles.

**PROF. G. PLATERO GOELLO**

Universidad Autónoma de Madrid, Spain

04-12 through 05-12-2003

Dynamical control of electronic states in AC-Driven Quantum Dots

**PROF. V. PONCE**

Centro Atómico Bariloche, Argentina

02-06 through 28-06-2002 and 02-06 through 30-06-2003

Electron emission in the interaction of light ions with surfaces.

Atomic Collisions In Solids. Ion-surface Interactions.



**DR. S. REICH**

Technische Universität Berlin, Germany

14-07 through 20-07-2003

Espectroscopia vibracional y absorción óptica en nanotubos y otros compuestos de carbono.

**DR. F. REINERT**

Universität des Saarlandes, Saarbrücken, Germany

18-04 through 21-04-2002

Photoemission study of the hole dynamics in surface states.

**PROF. D. RICHTER**

IFF-FZ, Forschungszentrum Jülich, Germany

07-07 through 14-07-2002 and 25-06 through 14-07-2003

Polymer dynamics by neutron techniques.

**PROF. A. SALIN**

Université de Bordeaux I, France

28-01 through 29-01-2002 and 03-02 through 04-02-2003

Dissociation dynamics of diatomic molecules at metal surfaces.

**DR. F. SCHILLER**

Universität Dresden, Germany

24-04 through 29-04-2003

Crystalline and electronic structure of thin Be and Mg films.

**DR. A. SCHNEIDER**

Max-Planck-Institut FKF, Stuttgart, Germany

17-04 through 19-04-2002

Scanning tunneling microscopy study of surface states.

**PROF. W.D. SCHNEIDER**

Université de Lausanne, Switzerland

10-10 through 13-10-2002

Scanning tunneling spectroscopy and microscopy of nanostructures.

**DR. W.D. SCHÖNE**

Free Universität Berlin, Germany

11-01 through 15-01-2003, 31-07 through 30-08-2003 and

14-12 through 18-12-2003

Lifetimes of excited electrons in metals.

Calculating quasiparticle energies in different approximations.

Many-body GW calculations of electronic structure and quasiparticle lifetimes in metals.

**DR. G. SCHWARTZ**

Chalmers University of Technology, Sweden

07-12 through 15-12-2003

General framework of dynamic properties of glass forming polymers by dielectric spectroscopy in combination with other experimental techniques and MD-simulations.

**DR. J. SJAKSTE**

Université Paris-Sud, France

08-09 through 09-09-2003

Electronic transfer in the interaction of ions with surfaces.

**PROF. J.M. SOLER TORROJA**

Universidad Autónoma de Madrid, Spain

31-01 through 01-02-2002

The SIESTA method for ab initio order-N materials simulation.

**PROF. P. SOUKIASSIAN**

Commissariat a l'Energie Atomique, Saclay, France

05-11 through 08-11-2002

Silicon carbide surfaces and nanostructures.

**PROF. M.J. STOTT**

Queen's University, Kingston, Ontario, Canada

13-07 through 16-07-2003

Modelling Bioactive Calcium Phosphate Ceramics.

**PROF. J. TEJADA PALACIOS**

Universidad de Barcelona, Spain

22-10 through 24-10-2003

Resonant spin tunnelling and related phenomena.

**PROF. S. TRETYAKOV**

Helsinki University of Technology, Finland

03-02 through 05-02-2003

Microwave technology and electron magnetic band gap materials.

**PROF. J.M. UGALDE URIBE-ETXEBARRIA**

Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain

14-02 through 14-02-2003

An innocent chemist look at the Density Functional Theory.

**S. VACCARO**

EPFL Lausanne, Switzerland

03-02 through 04-02-2003

Optical metamaterials in microwave technology.

**PROF. V.R. VELASCO**

ICMM-CSIC, Spain

12-12 through 13-12-2002

Physical properties of quasi-periodic systems. Dreams and realities.

**PROF. L. VIÑA**

Universidad Autónoma de Madrid, Spain

31-01-2002 through 31-01-2003 and 30-05 through 30-05-2003

Semiconductor quantum microcavities: a solid state approach for condensation.

**PROF. U. VON BARTH**

Lunds Universitet, Sweden

19-10 through 23-10-2002

Density functional theory and many-body approaches for exchange and correlation functionals.

**DR. M. WIERZBOWSKA**

Trinity College, Dublin, Ireland

16-06 through 06-07-2003

Ab-initio calculations in dilute magnetic semiconductors. Description of components based on GaN by means of an LDA+U approach.

**PROF. H. WINTER**

Technische Universität Wien, Austria

30-05 through 21-06-2002

Molecular projectile effects for kinetic electron emission from carbon- and metal surfaces bombarded by slow hydrogen ions.

**PROF. H. WINTER**

Universität zu Berlin, Germany

15-06 through 18-06-2002

Charge exchange, energy loss and electron emission in Ion-Surface Collisions.

**PROF. E. ZAREMBA**

Queen's University, Canada

21-07 through 06-08-2002

Bose-Einstein Condensate.

**DR. I. ZOZOULENKO**

University of Linköping, Sweden

05-09 through 06-09-2003

Wave and ray dynamics in optical cavities and quantum electron billiards.