AT-A-GLANCE

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OUR RESEARCHERS

AN INTERNATIONAL TEAM

The Foundation hosts long-term researchers which collaborate with visiting researchers on leading topics in Condensed Matter Physics and Polymer and Non-Crystalline Materials. The staff is international in origin; Croatia, France, Germany, Portugal, Russia, Sweden, and the USA. This is a feature of DIPC which reflects the very nature of modern scientific discovery. ■

Dr. S. Deutscher

COMING FROM Université de Paris-Sud. Orsay Cedex (France)
Laboratoires des Collisions Atomiques et Moleculaires (LCAM)

DATE 04/01/2000 through 09/15/2001

The following subjects are being studied:

- Investigation of metallic systems which are strongly perturbed by a heavy ion (Z>>1): it uses distorted wave functions to study in random phase approximation (RPA) the selfconsistent response of the metallic substrate to the perturbing ion and Auger transition rates in such systems.
- Investigation of interactions of slow ions with insulators. Focusses on charge exchange and energy loss phenomena during the interaction of slow ions with insulators.

These projects involve a Ph.D. student, several members of DIPC and of the Departamento de Física de Materiales of the Universidad del País Vasco/Euskal Herriko Unibertsitatea, as well as collaborators from France and Canada.

Dr. R. Díez Muiño

Member of Fellows Gipuzkoa: a program supported by Provincial Authority of Guipuzcoa

COMING FROM Lawrence Berkeley National Laboratory. California (USA)

ARRIVAL DATE 12/01/2000

Multiple Scattering in Non-Spherical Potentials (MSNSP) is used to calculate the angular distributions of electrons photoemitted from the 1s-shells of CO and N2 gas-phase molecules, with fixed-in-space orientations, as recently measured by several groups. For low kinetic energies of the photoemitted electrons (E<50 eV), as appropriate to certain shape-resonances, the electron scattering cannot be adequately represented by spherically-symmetric potentials. Hence we include non-spherical scattering potentials in our formalism through non-diagonal scattering matrices. The experimentally measured angular patterns, including those at the shape resonance energies, are accurately reproduced by our calculations.

Dr. S.V. Eremev

COMING FROM Institute of Strength Physics and Materials Science
Russian Academy of Sciences. Tomsk (Russia)

DATE 03/01 through 05/31/2000

For investigations of electron-phonon interactions on clean metal surfaces covered with adlayers of alkali atoms the quasi-one dimensional model has been developed. The key point of this model is the unscreened potential of a single atomic layer. This potential is constructed from the well known quasi-one dimensional screened model potential generated for thin films of many metals. The proposed single layer "ion" potential gives allow to calculate the transversal and longitudinal phonon modes and deformations potential and can be directly used for the calculation of the electron-phonon contributions the electronic lifetimes.

Prof. B. Gumhalter

COMING FROM Institute of Physics of the University Zagreb (Croatia)

DATE 11/01 through 12/31/2001

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.

- Asseessment 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 copuling 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.

Prof. B. Hellsing

COMING FROM Chalmers University (Sweden)
DATE 06/01 through 07/31/2001

Understanding of the temporal evolution of quasiparticles is of paramount importance to describe many important phenomena as the dynamics of charge and energy transfer, quantum interference, localisation and many others. It has been investigated the electron phonon interaction contribution to the lifetime of surface states on noble metals. The calculations, including the electron and phonon states of the bulk and surface, resolve the importance of the Rayleigh mode in function of temperature and binding energy of the surface electronic state.

Dr. A. Joukov

COMING FROM Institute of Solid State. Russian Academy of Sciences.
DATE 07/01/2000 through 12/31/2001

Recently studies of unidimensional magnetic materials (wires or fibers) become a topic of special interest owing to their unusual and exciting properties, such as giant magneto-impedance, magnetic bistability, elevated magnetic permeability etc. General tendency on the miniaturization of chips and sensors made from modern magnetic materials makes studies of tiny wires technologically attractive. Therefore the main attention has been paid to the study of tiny (1-50 ?m) amorphous and nanocrystalline wires.
The following problems have been studied:
- Magnetization Processes: Effect of chemical composition, applied stresses and sample geometry on magnetization curve, hysteretic properties and magnetostriction constant.
- Effect of the thermal treatments: structure and stress relaxation and nanocrystallization.
- Giant Magneto-impedance effect. Correlation of surface magnetic properties and high frequency transport properties.

Ph.D. students of UPV are involved in the development of the project.

Prof. V. Joukov

COMING FROM Institute of Solid State Chemistry.
Russian Academy of Sciences. Ekaterinbourg (Russia)
DATE 04/15/2000 through 12/31/2001

By using ab initio approaches LMTO-ASA and FP-LMTO the theoretical studies of the lifetimes of electrons excitations have been performed for Al, Cu, Ag, Au, Nb, Mo, Rh, Pd, Fe, Co, Ni. Basing on the scattering theory, a semiempirial physically transparent model has been proposed that explains the energy dependency of the averaged excitation lifetimes.

Dr. I. Koroteev

COMING FROM Institute of Strength Physics and Materials Sciences. Tomsk (Russia)
DATES 02/01through 04/30/2001 and 12/01/2001 through 12/31/2001

A necessary and important part of the adsorption theory must be a description of the electronic structure of clean surfaces and atoms when they are situated just outside the surface. As the first step of an investigation of interaction of alkaline metal atoms with metallic surfaces the electronic structure of clean vicinal surfaces has been studied. The one-dimensional model of a vicinal surface with noninteracting terraces of a varying width has been suggested. By using this model the electronic structure calculations of the Au(788) surface have been performed. It has been shown that the scattering of surface electrons by steps leads to the splitting of double degenerate surface states into the lateral confined states and into the states free propagating along terraces. Moreover the dependence of the confined level energies on the terrace width has been investigated. The spin-orbit coupling of surface states on vicinal surfaces has been considered too.

Dr. J. Kuntze

COMING FROM Institut für Experimentelle und Angewandte Physik der Universität Kiel (Germany)
DATE 06/04 through 12/31/2001

Our aim is to create and characterize lateral nanostructures using a combination of scanning tunneling microscopy (STM) in our local laboratory and photoelectron spectroscopy at synchrotron facilities. In the local lab, a UHV-system comprising a variable-temperature STM, LEED, evaporators and preparation facilities has been installed and tested. First experiments are focusing on vicinal surfaces of Si, Au and Cu. By deposition of Ag on vicinal Si a grid of one-dimensional structures can be grown which can be further used as a template for producing arrays of silver quantum dots. Growth of Ag on vicinal Au and Cu is currently under investigation. By lowering the substrate temperature we hope to change the growth conditions such that a self-assembly of Ag into an array of islands can be achieved as in the case of Co on Au. Besides fabrication and structural characterization of such nanostructures, the local electronic properties can be assessed by tunneling spectroscopy. Improved tip preparation facilities are being implemented to enhance the instrument's performance in that respect.

Dr. E. Leroy

COMING FROM Laboratoire de Materiaux Moléculaire, UMR CNRS. Lyon (France)
DATE 05/01 through 12/31/2001

Study and modelisation of the component segmental dynamics in miscible polymer blends using dielectric spectroscopy, particularcly in the case where only one component of the blend is dielectrically active, this component being either the one having the lower glass transition temperature (PVME in PVME/PS blends) or the higher one (PoCIS in PS/PoCIS blends).

Dr. C. Lorthioir

COMING FROM Laboratoire de Physique de Solides. Université Paris-Sud (France)
DATE 10/01 through 12/31/2001

Confining polymer chains within geometries of nanoscopic dimensions induces deep changes in their static and dynamic properties. The investigation of confinement effects is a challenging question of fundamental interest. In the current work, the self-confinement occurring in miscible blends of polystyrene (PS) and poly(vinyl methyl ether) (PVME), in the

high PS weight fraction regime ((PS (50%), is studied. Even though a single glass-transition temperature Tg is observed in these PS/PVME blends, the two components exhibit a strong difference in mobility, at the segmental level. Thus, close to Tg, the PS/PVME blends offer a good avenue to study fluid (PVME) chains three-dimensionally confined in a glassy (PS) matrix. The dynamics of the PVME segments is probed by broad band dielectric relaxation spectroscopy (10-3 - 107 Hz). On the other hand, neutron scattering techniques are used to characterise the structural properties of the confined systems (intermolecular structure of PS within the blends).

Dr. M. Marqués

COMING FROM Universidad de Coimbra (Portugal)
DATE 05/01through 12/31/2001

During the last years time-dependent density functional theory (TDDFT) emerged as one of the main tools to obtain excited-state properties in condensed-matter physics. It allows us to calculate linear quantities, like optical-absorption spectra, and also to tackle problems beyond the perturbative regime.
In this context, we investigate the response of molecules to light, including the calculation of optical and photo-electron spectra, photo-isomerisation, etc. We also research the interaction of systems with high-intense, ultra-short laser pulses, and the wealth of new and exciting phenomena related (high harmonic generation, above-threshold ionisation, etc.). Till now we have concentrated on small systems, like sodium, carbon and silicon clusters, but calculations of larger systems, including some biological molecules in currently under way. All these studies are performed within a real-space, real-time approach. At a more fundamental level, we test and try to improve on the exchange-correlation functional that exist in the market (these are the basic approximation in TDDFT).

Prof. I. Nagy

COMING FROM Technical University of Budapest (Hungary)
DATES 05/01 through 07/31/2000, 01/01 through 01/31/2001,
05/01 through 06/30/2001 and 09/01 through 10/31/2001

The work of Prof. Nagy during his stay at the DIPC has mostly focused on the theoretical study of the inelastic processes suffered by low-energy electrons in metals:

- Non-linear effects in the mean free path of low-energy electrons, by means of a scattering formalism. An effective particle-particle potential is used to describe the single-pair excitations.
- Spin effects in the lifetime of low-energy electrons, using first-order perturbation theory. The relative motion of the electrons, a kind of dynamical correlation effect, is included in the effective particle-particle potential.

The work of Prof. Nagy was developed in collaboration with M. Alducin, J. I. Juaristi, A. Arnau, and P. M. Echenique.

Dr. J. Osma

COMING FROM Universidad del País Vasco / Euskal Herriko Unibertsitatea (Spain)
Departamento de Física de Materiales
DATE 01/01 through 02/29/2000

Lifetimes of Surface States. A metal surface generates electron states that do not exist in a bulk metal. These so-called surface states can be classified into two categories, crystal-induced (intrinsic) states and image-potential-induced (image) states. Inelastic lifetimes are obtained from the knowledge of the quasiparticle self-energy, which we compute, within the

GW approximation of many body theory, by going beyond a free-electron description of the surface. Surface-state lifetimes in noble metal surfaces are presented. The results show that actual lifetimes are highly sensitive to the details of the surface response and to the presence of the intrinsic surface state itself.

Dr. V. Popov

COMING FROM General Physics Department. Altai Technical University. Barnaul (Russia)
DATES 03/01 through 05/30/2000 and 11/01/2000 through 01/31/2001

The self-consistent band structure Green's function meted has been developed for binary paramagnetic and ferromagnetic alloys with an arbitrary long-range order parameter, n. The calculations of band structure, density of states, the Fermi surface topology, and magnetic moments have been performed for bcc Fe, fcc Ni and the Ni-Fe alloys. It was shown that for partially disordered alloys ($n<1$) the energy bands have finite width due to the electron scattering on lattice sites occupied by different atoms with probability which is directly connected to stoichiometry of an alloy. In contrast to well known self-consistent coherent potential approximation (CPA) method the Green's function method takes explicitly into account the long-range order of alloys. It was shown that this effect leads to magnetic moment that depend on n.

Dr. M. Röesler

COMING FROM Hahn Meitner Institut. Berlin (Germany)
DATES 06/01 through 06/30/2001 and 09/01 through 09/30/2001

The work of Prof. Rösler has been focused on the theoretical study of the electrons emitted in the interaction of slow ions with metal surfaces. The kinetic electron yield collected when highly-charged N ions interact with Au surfaces has been analyzed. The performed calculations show that there is no significant dependence on the initial charge state of the ion.
Electron emission spectra of H projectiles moving inside Mg targets over a wide range of energies have been analyzed as well. The charge state of the projectile is theoretically calculated by including all posible charge-transfer processes between the projectile and the target.
The work of Prof. Rösler was developed in collaboration with R. Díez Muiño, J. I. Juaristi, and F. J. García de Abajo.

Dr. S. Silkine

COMING FROM Institute of Strength Physics and Materials Science
Russian Academy of Sciences (Russia)
DATE 02/01/2000 through 12/31/2001

The theoretical investigations of dynamics of quasiparticles in the surface and image potential states for clean noble (Cu,Ag,Au,Pt) and simple (Al,Be) metal surfaces as well as Cs covered Cu(100) and Cu(111) surfaces with the use of model potential and first principles pseudopotential approaches have been performed. The calculated linewidths of quasiparticle states are in good agreement with available STM and photoemissions experimental results. For the Cs/Cu(100) and Cs/Cu(111) systems the importance of L and X band gaps of bulk Cu for the long lifetime of the excited Cs induced transient states is shown. Also the frequency- and momentum-dependent dielectric function ((q,() has been calculated for intermetallic superconductor MgB2. Two plasmon modes were found at the energies (2 and (20 eV. For the (0001) surfaces of this material our ab initio calculations reveal a variety of very clear surface and subsurface states as well as resonance image-potential states with n=1,2.

Dr. M. Voda

COMING FROM INFM. Bucarest, Magurele (Rumania)

DATE 01/01 through 12/31/2001

The scientific activities developed during the year 2001 have been mainly involved with developing a new crystal growth method for the synthesis of KPb2CL5 crystals doped with rare earth. The method combine the purification of starting compounds by chlorination of molten chlorides with <one-melting and Bridgman single crystal growth techniques.
The results about the optical properties and potential applications of these materials have been published in the "2001 Joint International Meeting of the Electrochemical Society", Sept. 3, 2001 and in a paper accepted for publication in the "Journal of Luminiscence". Recent investigations on an Ytterbium doped KPb2CL5 crystal have shown internal laser cooling in this material for the first time.