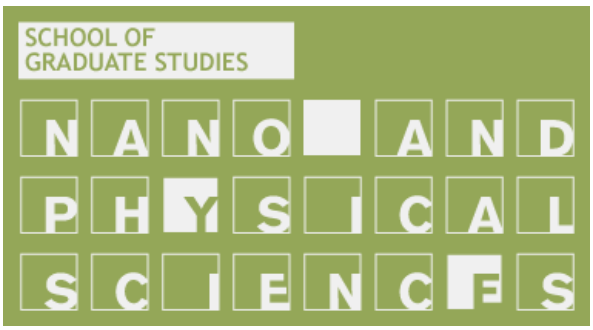


Proposal for a PhD Thesis 2009

Title: Quantum effects in molecular nanomagnets.

Proposer: Prof. Marco Affronte

Tutor: Prof. Marco Affronte

Type: Experimental

abstract: Molecular NanoMagnets have shown quantum phenomena at the macroscopic scale. Our group has recently proposed to exploit some functionalities of these molecules like the magnetocaloric effect (Appl. Phys. Lett. 87, 072504, 2005) or potentialities for the storage and processing quantum information (PRL 94, 207208 2005; PRL **97,** 207201 2006). The thesis work comprises the set up of low temperature experiments (e.g. magnetization under electromagnetic –MW, light- radiation, specific heat etc.) and the study of quantum phenomena (entanglement and superposition of quantum states) in a class of molecular nanomagnets (e.g. molecular antiferromagnetic cages, molecular tetrahedrons etc.).

Collaborations: Institut Néel CNRS Grenoble (F); Claredon Laboratory Oxford (UK); Dpt. Chemistry, Univ. Manchester (UK).

Coworkers: (at UniMORE): Dr. A. Candini; Dr. A. Ghirri.

Extra-bourse (15keuero/year) available: no

support for hosting foreign students (4Keuro/year) available: yes

supplementary information: http://www.s3.infm.it/line2_index.html

SCHOOL OF GRADUATE STUDIES

NANO AND PHYSICAL SCIENCES

Proposal for a PhD Thesis 2009

Title: Non-contact AFM investigation of oxide surfaces and metal clusters

Proposer: Dr. Stefania Benedetti

Tutor: Prof. Sergio Valeri

Type: Experimental

abstract:
Oxide surfaces have gained much interest in the last years because of their wide applications in catalysis and gas sensing devices. In particular the comprehension of the features at the atomic scale is fundamental to understand the behaviour of such surfaces when exposed to adsorbates. Non Contact (NC)AFM is a powerful tool to get insight into the defects and the atomic-scale mechanisms on the surface.
The aim of the proposed thesis is the preparation of oxide surfaces and the analysis by NC-AFM of the defectivity and its interplay with gas molecules and metal clusters adsorbed or nucleated on top of them. The activity includes also the improvement of the instrument to reach a good atomic resolution on various materials. The morphological investigation will be supported by other advanced techniques for surface investigation.

Collaborations:
Prof. M. Reichling, University of Osnabrueck, Germany
Prof. H.-J. Freund, Fritz Haber Institut, MPG, Berlin, Germany

Coworkers: (at UniMORE)
Dr. Paola Luches, Dr. Piero Torelli

Extra-bourse (15keuero/year) available: no

support for hosting foreign students (4Keuro/year) available: yes

supplementary information: www.sesamo.unimo.it

Proposal for a PhD Thesis 2009

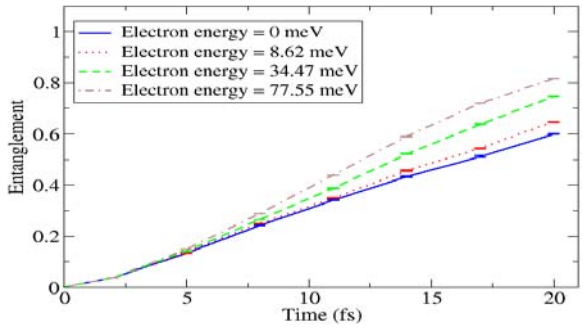
Title: Electronic decoherence in semiconductors

Proposer: Dr. Paolo Bordone

Tutor: Dr. Paolo Bordone

Type: Theoretical

abstract: The topic of this thesis is the analytical and numerical investigation of the entanglement dynamics of electrons interacting with other charges and/or with phonons in semiconductor systems. The Wigner Function approach can be used to study the mechanisms governing electronic decoherence in semiconductors for an electron subjected to an external electrostatical field or for various kind of electron-phonon interaction. Another possible development is the study of the entanglement appearing in the case of scattering of a single electron by few charges confined in a quantum dot, in connection with the experimental results obtained for the coherent components of the transmitted current in the case of multi-occupancy of a quantum dot.

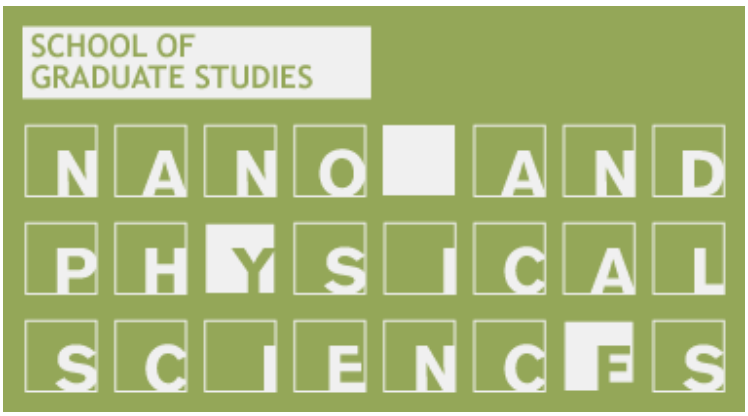


Time evolution of the entangelment between an electron and the the phonon bath of the crystal lattice at a temperature of 77 K for different electron energies

Collaborations:
Dr. F. Buscemi and Prof. M. Rudan, ARCES University of Bologna; Dr. A. Bertoni, S3 Research Center CNR-INFM; Prof. G. Compagno, University of Palermo.

Extra-bourse (15keuero/year) available: no

support for hosting foreign students (4Keuro/year) available: no



Proposal for a PhD Thesis 2009

Title: Monte Carlo simulation of electron transport in chalcogenide GST for applications to phase-change memory devices

Proposer: Rossella Brunetti

Tutor: Rossella Brunetti

Type: Theoretical

abstract: (no more than 800 characters)
Charge and heat transport properties of the chalcogenide GST material, suitably-modeled for describing phase-change memory devices, are presently the main focus of a number of research activities in view of the application of this material in nonvolatile-memory technology. The principle of chalcogenide memory was first proposed in the late 1960s by Ovshinsky who reported the observation of a reversible memory switching in chalcogenide materials. In the last years, semiconductor industries have considered the exploitation of the same concept for large-size, solid-state non-volatile memories, which nowadays seem to be very promising in terms of both performance and scalability perspectives.

The Monte Carlo simulation group of the Physics Department of the University of Modena and Reggio Emilia has been working on this subject since few years.

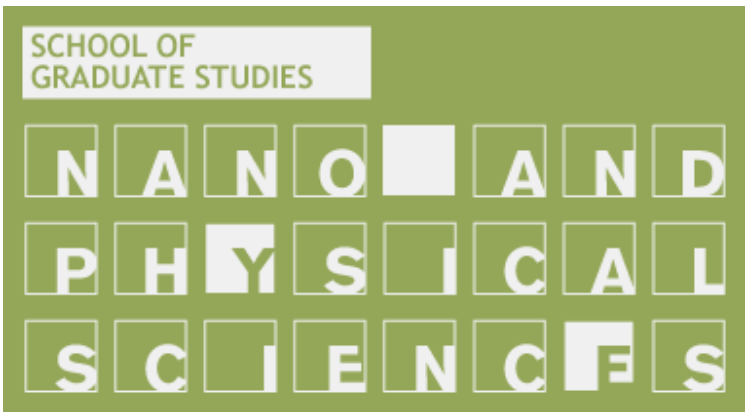
The proposed research aims at the production of an accurate, microscopic transport model for the carrier conduction in bulk amorphous GST, to be used in Monte Carlo simulations with the purpose of modeling the threshold voltage of a GST phase-change memory.

Collaborations: (other National or International groups directly involved in the research)
INTEL-USA

Coworkers: Carlo Jacoboni

Extra-bourse (15keuero/year) available: no

Support for hosting foreign students (4Keuro/year) available: no



Proposal for a PhD Thesis 2009

Title: Stretching proteins inside a computer

Proposer: Giovanni Bussi

Tutor: Elisa Molinari

Type: Theoretical

abstract: (no more than 800 characters)
Single-molecule measurements of mechanical stretching of proteins are a powerful experimental technique, as they can for instance be used to study the folding mechanism and to detect intermediate states. Furthermore, they allow for an experimental verification of the fundamental laws of non-equilibrium thermodynamics.
In the present thesis, the mechanical stretching of small proteins will be investigated *in silico* by means of atomistic molecular-dynamics simulations. Advanced techniques for the acceleration of rare events will be used, and if necessary new techniques will be developed. The work will be mainly based on computer simulations and on their comparison with experiments. The properties of the simulated systems will be also studied from the point of view of non-equilibrium thermodynamics.

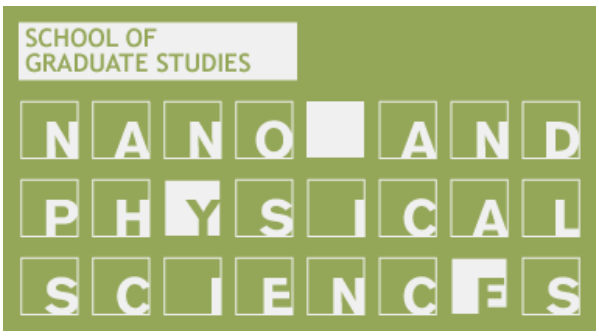
Collaborations: (other National or International groups directly involved in the research)

Coworkers: (at UniMORE)

Extra-bourse (15keuero/year) available: (yes/no)

support for hosting foreign students (4Keuro/year) available: (y/n)

supplementary information: (webpage address if available).



Proposal for a PhD Thesis 2009

Title: Phase Transition and Casimir Forces

Proposer: Carlo Calandra Buonaura

Tutor: Carlo Calandra Buonaura

Type: Theoretical/Computational

Abstract:

Extra-bourse (15keuero/year) available:

Support for hosting foreign students (4Keuro/year) available

Supplementary information:

Proposal for a PhD Thesis 2009

Title: Hybrid interfaces for photovoltaic applications

Proposer: Dr Arrigo Calzolari

Tutor: Dr. Alice Ruini

Type: Theoretical

Abstract: The aim of this thesis is the microscopic description of hybrid interfaces between organic molecules and oxide substrates for light harvesting and photovoltaic applications. The PhD activity will regard high-performance first principles calculations, based on static and time-dependent Density Functional Theory (DFT) approaches. This methodology allows one to describe the metastable atomic geometry and the corresponding electronic properties of the system, giving deep insights also into the optical and transport properties of the interfaces. The candidate will investigate a few realistic systems constituted of hybrid oxide/molecule and oxide/conductor interfaces. The focus will be on non-polar ZnO surfaces in connection either with natural organic dyes (anthocyanins) and with inorganic conducting surfaces (glass, transition metals). The former system is a good prototype for the optically active part of the solar cell, while the latter one allows one to describe the performance of the electrode contacts.

Collaborations: Dr. Alessandra Catellani (CNR-IMEM, Parma) [THEO]; Prof. Itamar Willner and coworkers (Institute of Chemistry, The Hebrew University of Jerusalem , Israel) [EXP].

Coworkers: (at UniMORE) Prof. Elisa Molinari, Dr. Daniele Varsano

Extra-bourse (15keuero/year) available: to be defined later

Support for hosting foreign students (4Keuro/year) available: to be defined later

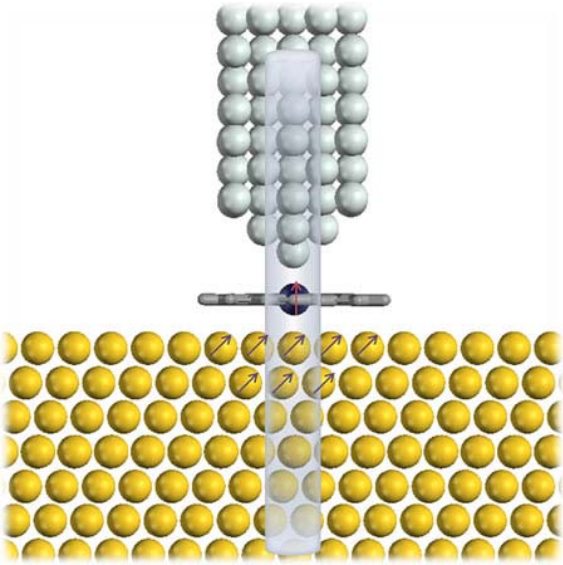
Supplementary information: www.nanoscience.unimore.it/pv.html
or contact calzolari.arrigo@unimore.it

SCHOOL OF GRADUATE STUDIES

NANO AND PHYSICAL SCIENCES

Proposal for a PhD Thesis 2009
Title: Electronic, optical and transport characteristics of hybrid interfaces
Proposers: Rosa Di Felice and Arrigo Calzolari
Tutor: Dott. Alice Ruini
Type: Theoretical/Computational
abstract:

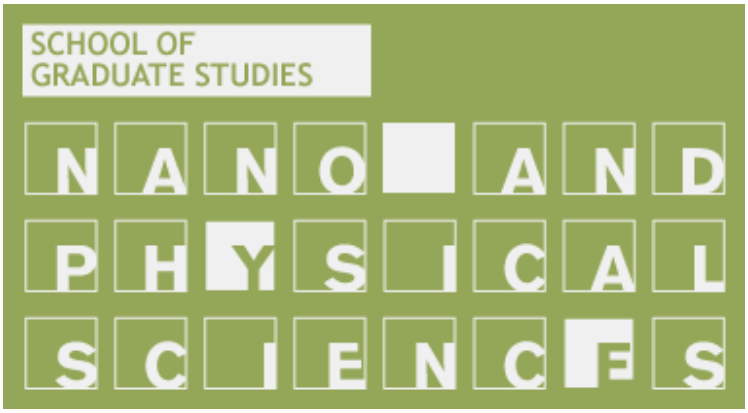
Hybrid interfaces, namely interfaces between materials of different natures, are attracting increasing attention in the context of nanosciences and nanotechnologies. We are interested in diverse classes of such systems, such as metal/semiconductor, molecule/surface and bio-molecule/polymer interfaces. The targets of our activities range from single-thiol molecules (thiolated DNA) and multiple-thiol polymers (MoSI wires) on metal surfaces, to planar molecules on metal subsrates, to metal/semiconductor coupling, to the hybridization of DNA oligomers with nanoparticles and organic polymers (MMX, MoSI) using different strategies (by H-bonding or chemical attachment). Spintronics systems are also considered. In all cases, we aim at understanding the mechanism and extent of the atomic and electronic coupling across the interface, and their significance in practical terms as well as self-assembling paradigms. The work is based on Density Functional Theory (DFT) electronic structure calculations and will require the use of different levels of theory, also beyond DFT (TDDFT, GW&Bethe-Salpeter).



Collaborations: (other National or International groups directly involved in the research)

1) Prof. M. G. Betti and Prof. C. Mariani (Università di Roma "La Sapienza") – EXP
2) Dragan Mihailovic, Jozef Stefan Institut (Ljubljana, Slovenia) – EXP
3) Rosangela de Paiva, Giorgia Brancolini, Daniele Varsano, Natl. Ctr. S3 of INFM-CNR (Modena, Italy) – THE
4) Felix Zamora&Julio Gomez, Universidad Autonoma de Madrid (Madrid, Spain) – EXP
5) Uri Banin, Hebrew University (Jerusalem, Israel) – THE

Coworkers: (at UniMORE) Prof. Elisa Molinari
Extra-bourse (15keuero/year) available: to be defined later
support for hosting foreign students (4Keuro/year) available: to be defined later
supplementary information: www.nanoscience.unimore.it
or contact rosa@unimore.it **or** calzolari.arrigo@unimore.it



Proposal for a PhD Thesis 2009

Title: Electron transfer processes in biological systems

Proposers: R. Di Felice, S. Corni (Research Center S3)

Tutor: E. Molinari

Type: Theoretical

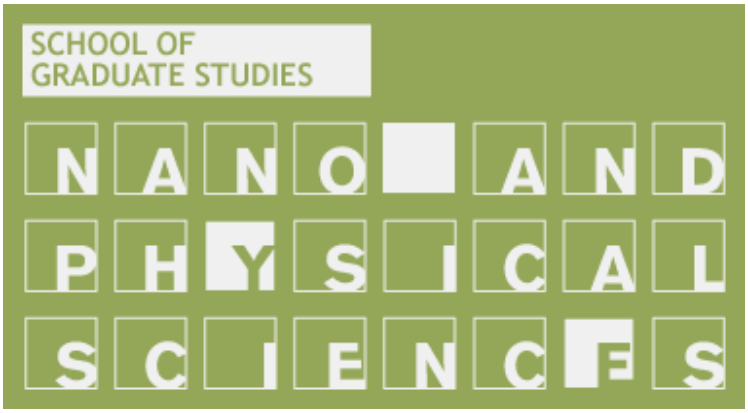
Abstract: (no more than 800 characters) The electron transfer (ET) between two biomolecular sites is of paramount importance in several biological processes, such as respiration or DNA oxidative damage. Recently, the interest in ET is even increased, thanks to the potential use of biomolecules in electronic devices (biomolecular electronics). Despite of its importance, very general issues in bio-ET are still open. For example, ET over long distances can take place via different mechanisms, with different practical consequences. Also the ET between a biomolecule and a metal electrode, the interface between the bio(nano) world and the macroscopic one, is poorly understood due to the complexity of the system. These issues will be tackled via state-of-the-art computational tools, such as quantum-mechanical simulations and classical molecular dynamics. This thesis requires much computer work, but may include theoretical development and software implementation.

Collaborations: The research project will be developed in collaboration with experimental groups at S3 (Paolo Facci), previous group members (Agostino Migliore, Center for Molecular Modeling, University of Pennsylvania, USA) and other important international groups (Joshua Jortner, School of Chemistry, Tel Aviv University)

Coworkers: (at UniMORE)

Extra-bourse (15keuero/year) available: (yes/no)
Supporting funds will be defined later.

support for hosting foreign students (4Keuro/year) available: (y/n)
Supporting funds will be defined later.
supplementary information:
http://www.s3.infm.it/prosurf
http://www.nanoscience.unimore.it/stefano.html
http://www.nanoscience.unimore.it/rosa.html



Proposal for a PhD Thesis 2009

Title: Bio-inorganic surfaces: Simulating the interaction between inorganic surfaces and proteins.

Proposers: S. Corni, R. Di Felice (Research Center S3)

Tutor: E. Molinari

Type: Theoretical

Abstract: (no more than 800 characters) Recent combinatorial biotechnologies have shown that the molecular recognition capability of proteins can be specifically oriented toward inorganic surfaces. Such specificity could lead to the elaboration of new technologies in several fields, from nanoelectronics to biomaterials. However, the principles regulating protein-surface interactions are poorly understood: What features of the surface and of the proteins determine which protein is able to bind to a given surface and how? The aim of this thesis is to theoretically address protein-surface interactions, applying and extending the tools of computational physics/chemistry/biology. In particular, a multiscale approach involving Quantum-Mechanics, Molecular Dynamics and docking-like techniques will be used. This thesis requires much computer work, but leaves space to theoretical development of methods for interfacing quantum and classical calculations.

Collaborations: The research project will be developed in collaboration with important European groups having different backgrounds (experimental and theoretical, chemically, physically and biologically oriented): Weizmann Institute of Science (Israel), EML Research (Heidelberg, Germany), Ludwig Maximilians University (Munich, Germany).

Coworkers: (at UniMORE)

Extra-bourse (15keuero/year) available: (yes/no)
Supporting funds will be defined later.
support for hosting foreign students (4Keuro/year) available: (y/n)
Supporting funds will be defined later.
supplementary information:
http://www.s3.infm.it/prosurf
http://www.nanoscience.unimore.it/stefano.html
http://www.nanoscience.unimore.it/rosa.html

Proposal for a PhD Thesis 2009

Title: Single Molecule Magnets at Surfaces

Proposer: Prof. Andrea CORNIA

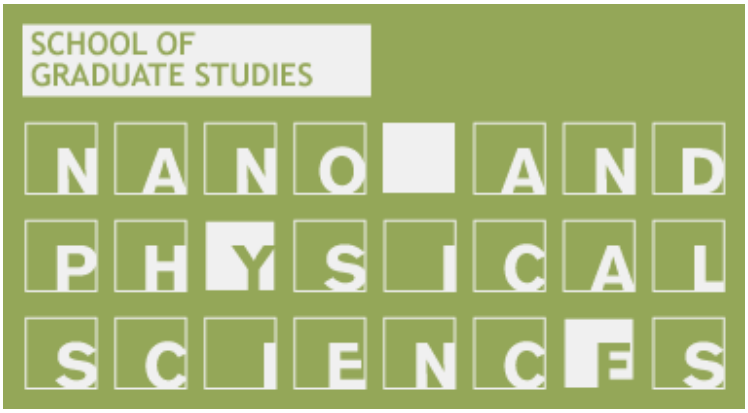
Tutor: Prof. Andrea CORNIA

Type: Experimental (Chemistry)

Abstract: (no more than 800 characters) Single Molecule Magnets (SMM) are metal-ion clusters displaying magnetic hysteresis at low temperature. They are studied as miniaturized units for information storage and processing in the framework of *molecular spintronics*, which requires to probe the response of individual molecules. Three approaches are currently followed: (1) attachment of magnetic molecules to carbon nanotubes in nanotube-based SQUID devices; (2) use of scanning probe techniques to address SMM on surfaces; (3) wiring of individual SMM to nanoelectrodes to give miniaturized electronic devices. The proposed research activity targets the design and synthesis of functionalized SMM suitable for the above-mentioned studies, to be carried out in collaboration with leading european groups in molecular spintronics.

Collaborations: (other National or International groups directly involved in the research)
Herre van der Zant: realization of single-molecule devices and electron transport measurements (Kavli Institute of Nanoscience, Delft University of Technology, Delft, The Netherlands)
Maarten Rolf Wegewijs: theoretical work (Institut fuer Theoretische Physik A, RWTH-Aachen, Germany)
D. Gatteschi, *A. Caneschi, R. Sessoli*: long-standing collaborators for magnetic studies (Laboratory of Molecular Magnetism, University of Florence, Florence, Italy).
*W. Wernsdorfer***:** nanotube-based SQUIDs (Laboratoire Néel – CNRS, Grenoble, France).
A.-L. Barra: High-frequency EPR (Grenoble High Magnetic Field Laboratory – CNRS, Grenoble, France)
Coworkers: (at UniMORE)
Dr. Chiara Danieli, post-doctoral fellow (design and synthesis of SMM)
Dr. Corrado Sciancalepore, PhD student (scanning probe microscopies and surface analysis)
Extra-bourse (15keuro/year) available: NO
Support for hosting foreign students (4Keuro/year) available: NO

Supplementary information: (webpage address if available).
http://155.185.2.170/sitiwebgruppi/Cornia/cornia_home.htm



Proposal for a PhD Thesis 2009

Title: *Multi-technique investigation of isolated single molecule magnets grafted on surfaces.*

Proposer: Dr. Valdis Corradini
Tutor: Prof. Marco Affronte
Type: Experimental

abstract: Single Molecule Magnets (SMM) have shown very interesting magnetic properties at the molecular level. They can be used to build up physical bit of future computers based on quantum-computation or for high density data storage. However, their exploitation need addressing single molecules, so it is crucial to be able to graft them onto suitable surfaces preserving their properties. The thesis work will be focused on the optimisation of new strategies for the controlled deposition of functionalized SMM on surfaces and their structural, electronic and magnetic investigation. The topology and chemistry of the SMM will be studied, on-campus, using Scanning Tunnel Microscopy and Electronic Spectroscopies, while the electronic and magnetic properties by X-ray Absorption and Dichroism at the Sinchrotron Radiation facilities.

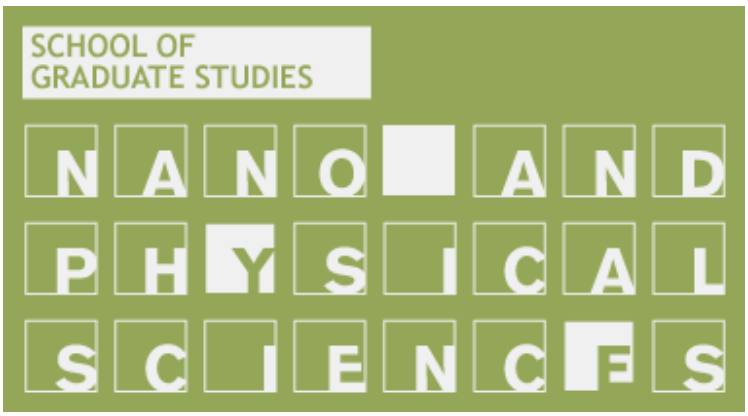
Collaborations: Prof. R. Winpenny, University of Manchester (UK); Dr. E. K. Brechin, "School of Chemistry" University of Edinburgh (UK); Prof. J. Veciana, Institut de Ciencia de Materials (CSIC) de Barcelona (ES); Prof. E.Coronado Instituto de Ciencia Molecular (ICMol), Universidad de Valencia (ES).

Coworkers: (at UniMORE) Prof. U. del Pennino, Dr. V. De Renzi, Dr. R. Biagi, Prof. M. Affronte Dr. A. Ghirri.

Extra-bourse (15keuero/year) available: no

support for hosting foreign students (4Keuro/year) available: Yes

supplementary information: http://www.s3.infm.it/surfnanomagnets_index.html



Proposal for a PhD Thesis 2009

Title: Production and characterization of magnetic cluster films

Proposer: Sergio D'Addato

Tutor: Sergio D'Addato

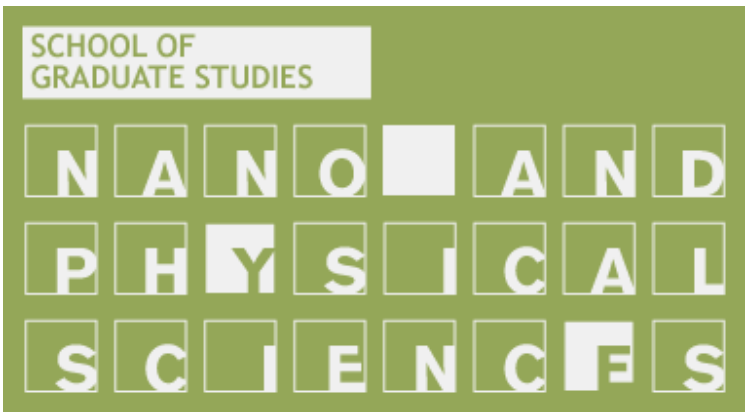
Type: (Theoretical/Experimental) Experimental

abstract: (no more than 800 characters)
The interest in metal nanostructured films has grown in the last years because of their fascinating physical properties and their potentiality in various applications, like magnetic recording industry, catalysis and tribology. We propose a PhD thesis devoted to the investigation of magnetic nanoparticle granular films obtained with a recently developed source which is able to produce and mass-select clusters. The study will be focused on the influence of size, thickness and volume fraction (when particles are codeposited with other metals) on the magnetic properties of the film. Some of the techniques to be used in campus will be AFM-STM, XPS, and MOKE. Part of the experimental activity will be also carried out in external facilities like synchrotrons (for PEEM and XMCD experiments), ain collaboration with other groups.

Collaborations: (other National or International groups directly involved in the research)
Federico Spizzo, at the Dipartimento di Fisica, Università di Ferrara.
Chris Binns, University of Leicester, UK (synchortron radiation experiments)
Monica de Simone, Cinzia Cepek at TASC (Trieste)

Coworkers: (at UniMORE)
A. di Bona, INFM/CNR, S3 research centre
Extra-bourse (15keuero/year) available: (yes/no) no
support for hosting foreign students (4Keuro/year) available: (y/n) yes

supplementary information: (webpage address if available). **http://www.sesamo.unimo.it, http://www.s3.infm.it**



Proposal for a PhD Thesis 2009

Title: Study of the single particle and collective excitations in Graphene

Proposer: Umberto del Pennino

Tutor: Umberto del Pennino

Type: Experimental

abstract:

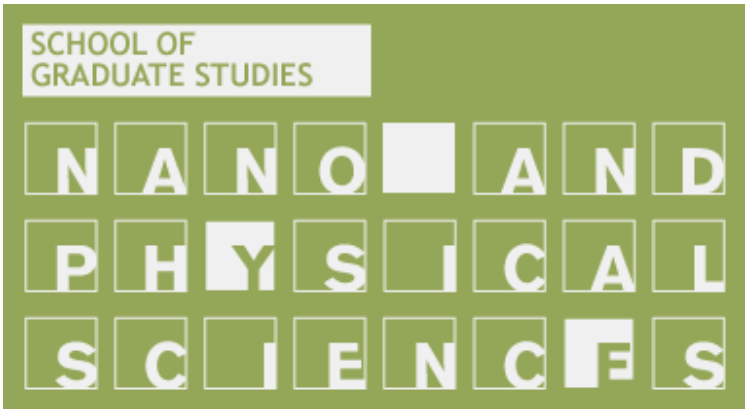
Graphene, an atomically thin layer of carbon atoms arranged in a honeycomb lattice, has attracted a lot of research interest because of its intriguing physics as well its application potential. The band structure of graphene exhibits two bands intersecting at two inequivalent points in the reciprocal space, K and K_0. Near these points, the electronic dispersion resembles that of relativistic Dirac electrons. When a multi-layer graphene sheet is grown on SiC it exhibits an energy gap at K and K_0, dependent on the layer thickness. We intend to produce single and multi-layer graphene layers on SiC or Ni in UHV and measure their electronic properties, in particular the gap opening, single particle and collective excitations by High Resolution Electron Energy Loss Spectroscopy.

Collaborations:

Coworkers: (at UniMORE)
Roberto Biagi
Valentina De Renzi
Valdis Corradini (INFM-S3)

Extra-bourse (15keuero/year) available: no

support for hosting foreign students (4Keuro/year) available: no



Proposal for a PhD Thesis 2009

Title: S*urface functionalization and nanostructuring of cantilever-based sensors*

Proposer: Dr. Valentina De Renzi

Tutor: Dr. Valentina De Renzi

Type: Experimental

Abstract:

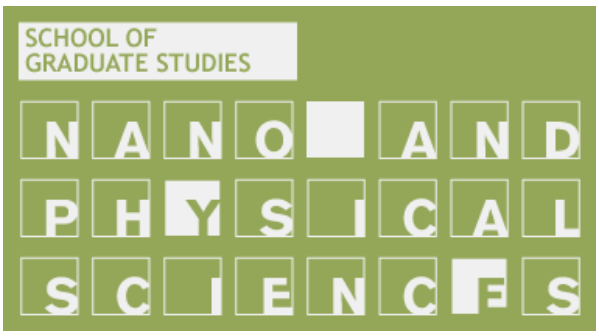
Molecular detection based on micro and nano cantilevers (CL) is currently deserving great attention both in fundamental science and in more applicative fields. Detection of specific molecular species relies on the local functionalization of the CL surface with organic adlayers, which are able to specifically interact with the target molecule. For an effective exploitation of CLs, a deeper comprehension of fundamental mechanics and chemistry of the molecular recognition process is needed. In the proposed PhD work, novel routes to functionalization will be addressed and the interface properties studied by means of surface science techniques (XPS, HREELS, LEED, STM, AFM). The influence of the adlayer mechanical and structural properties on CL detection will be investigated. Moreover, FIB-nanostructuring will be also performed to improve CL performances. Both CL of reduced dimensions and with novel shapes will be considered.

Collaborations: (other National or International groups directly involved in the research)
Dr. C. Ricciardi and Dr. G. Cicero Politecnico Torino (PoliTO), Dr. L. Nasi IMEM -CNR Parma, Dr. R. Felici ESRF – Grenoble - France

Coworkers: (at UniMORE & S3) Dr. G. Gazzadi ,Prof. U del Pennino, Dr. R. Biagi, Dr. V. Corradini,

Extra-bourse (15keuero/year) available: yes
support for hosting foreign students (4Keuro/year) available: yes

supplementary information: contact Dr. De Renzi for further information



Proposal for a PhD Thesis 2009

Title: Electronic structure and dynamics of DNA-derivatives for nanotechnology

Proposer: Rosa Di Felice & Daniele Varsano

Tutor: Elisa Molinari

Type: Theoretical/Computational

Abstract: Within the worldwide efforts towards self-assembling nano-electronics and nano-technology, DNA is particularly fascinating, also because of the biological interest of electron transfer through nucleobase stacks. In this context, we investigate the electronic structure and electron transfer properties, the stability, and the optical properties of synthetic DNA-based assemblies, also in contact with inorganic substrates. The target systems include: double-stranded DNA, M-DNA (DNA-metal complexes), G4-DNA (guanine quadruple helices), xDNA (aromatic expansion). The applied methods range from *quantum* calculations by Density Functional Theory (DFT electronic structure) and time-dependent DFT (optical absorption and circular dichroism), to *classical* molecular dynamics simulations. The activities are in successful collaboration with theoretical and experimental international groups.

Collaborations: (other National or International groups directly involved in the research)
Danny Porath (Dept. Physical Chem., Hebrew University of Jerusalem, Israel) – experiment
Angel Rubio (Udiversidad del Pais Vasco San Sebastian, Spain) – theory
Alexander B. Kotlyar (Dept. Biochem., Tel Aviv University, Israel) – experiment
Steen Nielsen (Dept. Phys.&Astron., Univ. Aarhus, Denmark) – experiment
Stefano Corni & Giorgia Brancolini (Natl. Ctr. S3 of INFM-CNR, Modena, Italy) – theory
Agostino Migliore (Dept. Chem. Univ. of Pennsylvania, Philadelphia, USA) – theory

Coworkers: (at UniMORE) Elisa Molinari

Extra-bourse (15keuero/year) available: to be defined later

Support for hosting foreign students (4Keuro/year) available: to be defined later

Supplementary information:
URL http://dna-nanodevices.s3.infm.it, www.s3.unimo.it
Email rosa@unimore.it, varsano.daniele@unimore.it

Proposal for a PhD Thesis 2009

Title: Ion channels-membrane interactions studied by high resolution/affinity imaging Scanning Probe Microscopy (SPM)

Proposer: Prof. Paolo Facci, Prof. Andrea Alessandrini

Tutor: Prof. Elisa Molinari

Type: Experimental

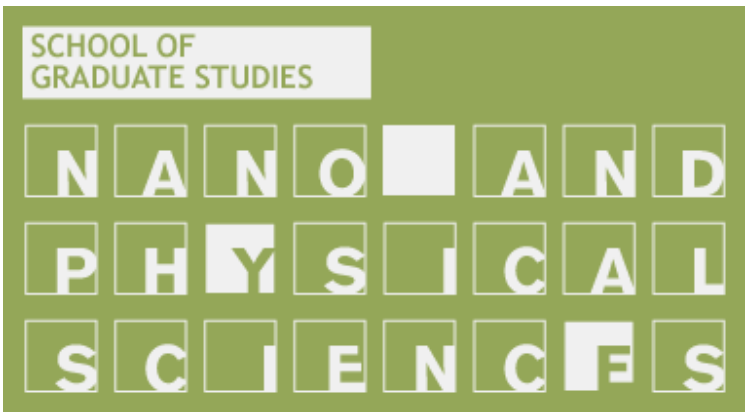
abstract:

In the proposed research activity the interaction of different membrane proteins with model membranes will be studied by high resolution SPM and affinity imaging with functionalized tips. The distribution of membrane proteins in model membranes will be studied as a function of the physical state of the bilayers. Different physical states in the bilayers will be induced by altering physical and chemical parameters (temperature, pH, ionic strength etc.) and imaged in real-time by SPM techniques. A temperature-controlled SPM will be exploited to study in real-time phase transitions in the bilayer and the consequent distribution rearrangement of membrane proteins. Also the functional properties of the ion-channels will be studied as a function of the membrane physical state by the BLM technique. SPM imaging of reconstituted ion-channels in the case of voltage-gated ion channels will be realized as a function of the transmembrane voltage drop.

Ref: Microscopy Research and Technique, 71, 274, 2008. Alessandrini A, Gavazzo P, Picco C, Facci P.

Coworkers: Heiko Seeger, Carlo Agusto Bortolotti

Extra-bourse (15keuero/year) available: yes (available for the first year)
support for hosting foreign students (4Keuro/year) available: no
supplementary information: www.biophysics.unimo.it

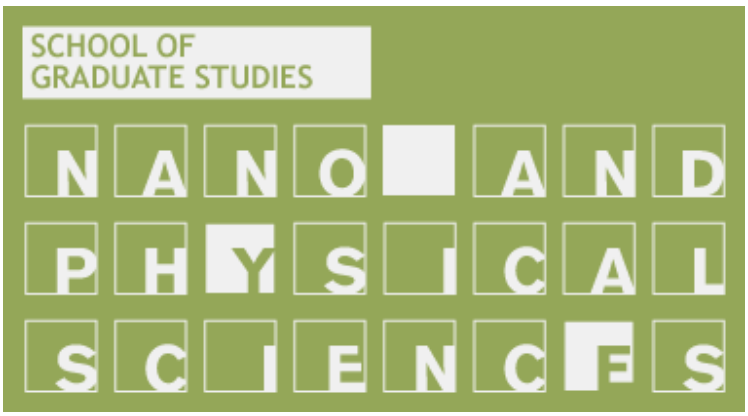


Proposal for a PhD Thesis 2009

Title: A multi-scale approach to semiconductor nanostructures: including interface states in k.p theories

Proposers:
Dr. Rita Magri, Dipartimento di Fisica, Università of Modena and Reggio Emilia
Dr. Guido Goldoni, Dipartimento di Fisica, Università of Modena and Reggio Emilia
Tutors:
Dr. Rita Magri, Dipartimento di Fisica, Università of Modena and Reggio Emilia
Dr. Guido Goldoni, Dipartimento di Fisica, Università of Modena and Reggio Emilia

Type: (Theoretical/Experimental)
Theoretical
abstract: (no more than 800 characters)
Present nano-technologies allow to grow systems with very high surface/volume ratio (nanoclusters, short-period superlattices, etc). Although interface states may strongly influence or even dominate their electronic properties (and ensuing optical properties or transport characteristics), they are elusive within present theoretical approaches. Indeed, such systems are too large to be treated by the computationally intensive atomistic methods; on the other hand, macroscopic methods, such as the k.p approach can easily treat nanosized materials but neglect the atomic details and surface states.
In this thesis, we propose a multi-scale approach which *combines atomistic and semi-empirical methods* to include interface localized states within a macroscopic approach. This will be achieved deriving a class of effective interface potentials to be used within the k.p class of theories.
A protocol will be defined for the definition of an optimal *transferable interface potential* for any pair of given classes of materials (particularly for the technologically relevant III-V materials, as, e,g, GaAs, InP, GaN, GaSb), independent from other structural parameters.
The project implies the extensive use of state-of-the-art atomistic packages, the k.p package NextNano3, and implementation of multi-dimensional optimization with artificial intelligence techniques.
Collaborations: (other National or International groups directly involved in the research)
Nextnano authors (Munich, Germany)
Coworkers: (at UniMORE)
Extra-bourse (15keuero/year) available: (no)
support for hosting foreign students (4Keuro/year) available: yes
supplementary information: (webpage address if available).
www.nanoscience.unimore.it; acmnew34.unimore.it



Proposal for a PhD Thesis 2009

Title: Optical excitations of hybrid molecular-semiconductor systems for photovoltaic applications: a new multi-scale approach

Proposer: Guido Goldoni, University of Modena and Reggio Emilia

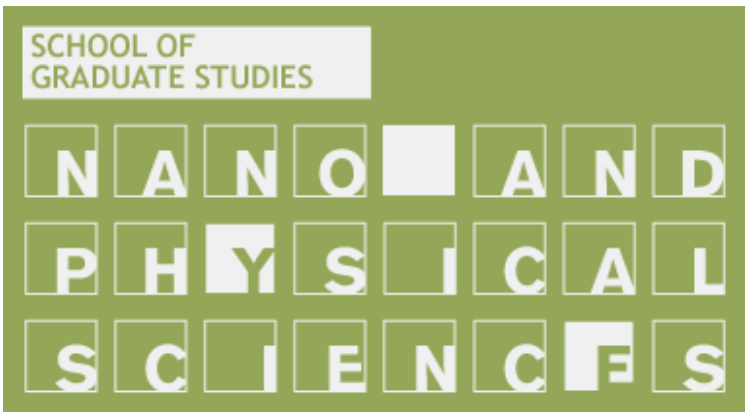
Tutor: Guido Goldoni, University of Modena and Reggio Emilia
Stefano Corni, CNR-INFM S3, Modena

Type: Theoretical

abstract: (no more than 800 characters)
New perspectives arise for photovoltaics as well as for other applied fields (diagnostics, drug delivery) from hybrid systems composed of organic molecules and inorganic semiconductor nanoparticles (quantum dots, QDs). At present no theoretical approach is available to describe the interaction of such systems with light, the main problem being that they are composed of sub-systems with very different, yet coupled, light-induced excitations; computational methods proper for molecules are computationally prohibitive for QDs, while standard methods used for QDs are by construction unsuitable for molecules.
The aim of this thesis is to develop a new theoretical description and ensuing codes based on a genuine multi-scale approach, combining two approaches suited to the separated sub-systems. The project will permit to get familiar with the physics of excitations of organic molecules, the optical properties of semiconductors and physics of hybrid interfaces. Technical skills will be acquired by use of state-of-the art molecular codes as well as specialized codes for semiconductor nanoparticles.

Collaborations: (other National or International groups directly involved in the research)
M. Caldas, Universidade de Sao Paulo, Brazil
Coworkers: (at UniMORE)
E. Molinari, University of Modena and Reggio Emilia

Extra-bourse (15keuero/year) available: to be defined
support for hosting foreign students (4Keuro/year) available: to be defined
supplementary information: (webpage address if available).
www.nanoscience.unimore.it



Proposal for a PhD Thesis 2009

Title: Optics and Quantum-Optics in Semiconductor Nanostructures

Proposer: Guido Goldoni, University of Modena and Reggio Emilia

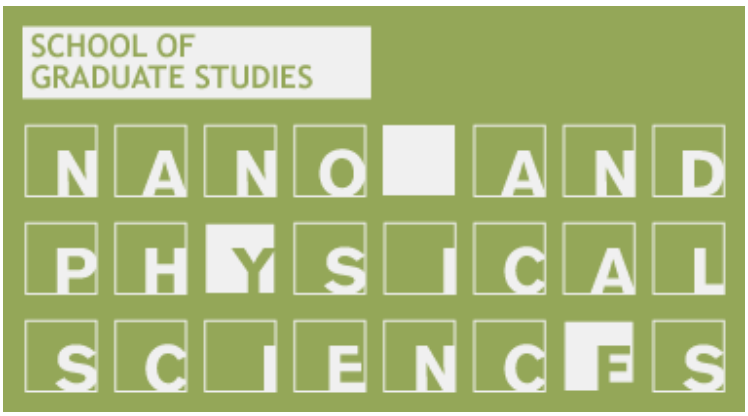
Tutor: Guido Goldoni, University of Modena and Reggio Emilia
Filippo Troiani, CNR-INFM S3

Type: Theoretical

abstract: (no more than 800 characters)
Semiconductor quantum nanostructures have unique optical properties which can be designed on purpose to a high degree. Quantum dots, carbon-based materials and nanowires are systems of specific interest for this thesis. Much of the interest is driven by the possible use of nanostructure-cavity systems as fundamental building blocks for quantum-information devices and generation of genuine quantum states for quantum-communication protocols (teleportation). In this perspective, we have been recently working at different schemes for generating indistinguishable single photons on demand, as well as entangled-photon pairs. The investigations will include i) simulation of (multi-)exciton states (energy, recombination rates, etc) in semiconductor nanostructures; ii) development of the schemes for indistinguishable photon generation and entangled states; ii) design and simulation of quantum structures for quatum-optica. Theoretical tools will include macroscopic (envelope function) theories of the electronic states, master equations schemes and development of artificial intelligence-based optimization tools.

Collaborations: (other National or International groups directly involved in the research)
C. Tejedor, Universidad Autonoma, Madrid
J. I. Climente, Universitat Jaume I, Castello, Spain
Coworkers: (at UniMORE)
Extra-bourse (15keuero/year) available: to be defined
support for hosting foreign students (4Keuro/year) available: to be defined

supplementary information: (webpage address if available).
www.nanoscience.unimore.it



Proposal for a PhD Thesis 2009
Title: Quantitative analysis of strain and composition in nanostructures by transmission electron microscopy techniques
Proposer: Dr. Vincenzo Grillo
Tutor: Prof. Stefano Frabboni
Type: Experimental
Abstract: Transmission Electron Microscopy (TEM) is an important tool for the analysis of materials and nanostructure down to the atomic scale. The possibility of different electro optical configurations makes it possible to perform by TEM both direct space imaging and reciprocal lattice analyisis. Moreover the continuously evolving fabrication technology and the use of more powerful controlling and analysis software have made the instrument very powerful and the field of its application very wide. It is possible, for example, to visualize a single doping atoms in a semiconductor, produce maps of the elastic strain or of magnetic fields, produce a tomographic maps of the shape of a nanoparticle.
The PhD activity in this field can be concentrated on both advanced simulation/analysis and or experimental activity depending on the aptitude of the student. The methodological study will be applied to different nanostructures in the field of semiconductors and magnetic materials.
Collaborations: TEM group @IMEM-CNR (Parma)
Supplementary information: Contact Dr. V.Grillo for further information. A web site will be also soon available by browsing inside www.s3.infm.it site

SCHOOL OF GRADUATE STUDIES

NANO AND PHYSICAL SCIENCES

Proposal for a PhD Thesis 2009

Title: Metal/oxide nanoparticles for catalytic applications

Proposer: Paola Luches

Tutor: Sergio Valeri

Type: (Theoretical/Experimental) experimental

Abstract: (no more than 800 characters)
Catalytic materials are very important for our daily life, for example to reduce the amount of pollutants emitted by car engines and factories. Most catalysts are made of supported metal or oxide nanoparticles. The proposed activity aims at the design of new catalytic materials with improved performances, through the understanding of the atomic-level physical and chemical properties of the nanoparticles and of their influence on the catalytic activity and selectivity. The student will make use of advanced techniques for the production of metal/oxide nanoparticles and for their characterization before, during and after the reaction (e.g. high resolution imaging by scanning probes, photoelectron spectroscopy and mass spectrometry). The activity involves also experiments at synchrotron radiation facilities.

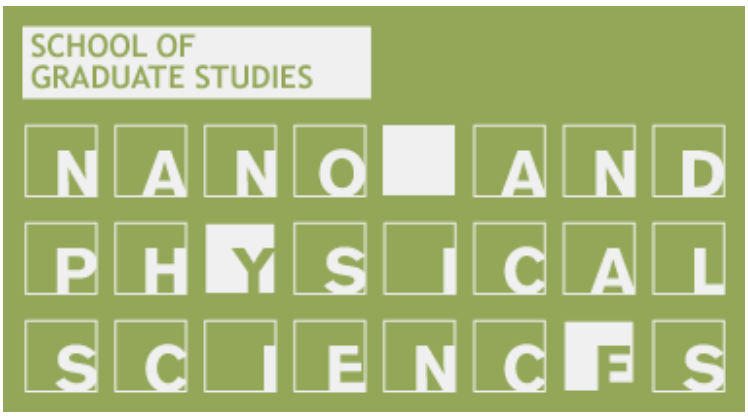
Collaborations: (other National or International groups directly involved in the research)
Falko Netzer, University of Graz, Austria
Jozef Korecki, Institue of Catalysis and Surface Chemistry, Krakow, Poland

Coworkers: (at UniMORE)
Stefania Benedetti (post-doc), Piero Torelli (researcher)

Extra-bourse (15keuero/year) available: (yes/no) no

support for hosting foreign students (4Keuro/year) available: (y/n) yes

supplementary information: (webpage address if available).



Proposal for a PhD Thesis 2009

Title: Ab-initio formalism for optical gain in silicon nanosystems

Proposers: Stefano Ossicini and Rita Magri

Tutors: Rita Magri and Stefano Ossicini

Type: (Theoretical/Experimental) Theoretical

abstract: (no more than 800 characters)
The comprehension of optical gain in Silicon nanocrystals (Si-nc) represents a first step toward a silicon laser. In this contest theory plays a fundamental role. In this thesis we aim at describing the electronic excitations of complex systems with efficient and accurate numerical simulations. Going beyond the state of the art, we intend to develop a formalism within the Bethe-Salpeter and Time-Dependent Density Functional Theory approaches, to examine the competing dynamical processes involved in optical amplification and lasing in Si-nc. This goal will be realized by solving a set of channel-specific rate equations, describing the dynamic of free and interacting carriers under a pump pulse, with characteristic recombination rates calculated within ab-initio schemes. The development of an ab-initio optical gain theory is crucial in order to determine the best conditions for lasing in Si-nc systems.

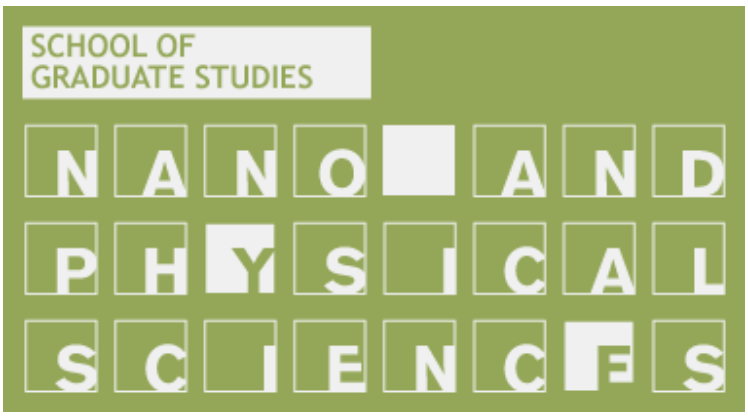
Collaborations: (other National or International groups directly involved in the research)
Dott.ssa O. Pulci, Universita' di Roma Tor Vergata (Theory)
Dott.ssa Lucia Reining, Ecole Politechnique, Paris (France) (Theory)
Prof. Lorenzo Pavesi, Universita' di Trento (Experiments)

Coworkers: (at UniMORE)
Ivan Marri, Roberto Guerra, Elena Degoli

Extra-bourse (15keuero/year) available: (yes/no)
No

support for hosting foreign students (4Keuro/year) available: (y/n)
Maybe

supplementary information: (webpage address if available).
acmnew34.unimore.it (provvisoria)



Proposal for a PhD Thesis 2009

Title: Modelli multiscala per lo studio della crescita epitassiale di nanostrutture semiconduttrici

Proposer: Rita Magri

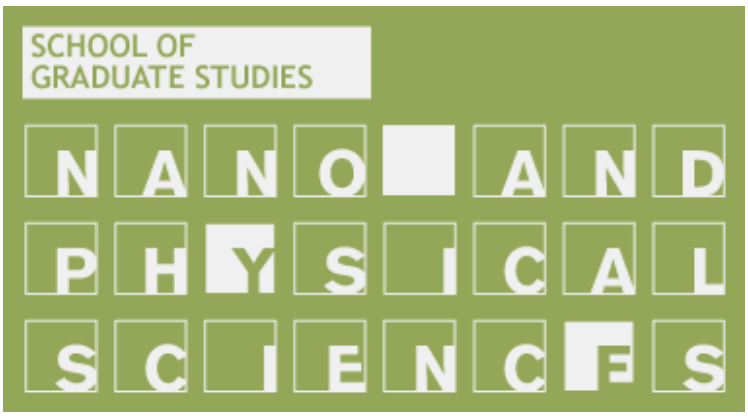
Tutor: Rita Magri

Type: (Theoretical/Experimental) Theoretical

abstract: (no more than 800 characters)
In hetero-epitaxial growth, e.g. of InAs on GaAs substrate, the nanoscale InAs nucleate at essentially random positions on the substrate surface. The essential randomness of the nucleation process poses limits to the homogeneity of the overall quantum dot ensemble produced, and in this way restricts the potential applications of these quantum dots, e.g. for semiconductor heterostructure lasers. There are some reports in the literature about preferential quantum dot nucleation near atomic-scale steps on the substrate. This effect could be exploited to improve the spatial arrangement of the quantum dots on the substrate, but its physical origin is still not fully understood. The goal of the present project is an improved understanding of the interaction of nanoscale hetero-epitaxial islands with surface steps, and develop improved capabilities for modelling semiconductor hetero-epitaxy in general. In terms of methodology, our aim is to develop efficient multi-scale modelling techniques that enable us to address the above questions.

Collaborations: (other National or International groups directly involved in the research)
Prof. Peter Kratzer, Universitat Duisburg-Essen - Fachbereich Phyzik, Lotharstrasse, 1 Duisburg 47048 Nordhrein-Westfalen (Theory)
Prof. Fulvia Patella, Prof. Adalberto Balzarotti, Dipartimento di Fisica, Università di Roma Tor Vergata (Experiments)

Coworkers: (at UniMORE)
Marcello Rosini
Extra-bourse (15keuero/year) available: (yes/no)
no
support for hosting foreign students (4Keuro/year) available: (y/n)
possible for one year
supplementary information: (webpage address if available).
acmnew34.unimore.it
www.nanomodelling.unimore.it



Proposal for a PhD Thesis 2009

Title: Semiconductor nanowires for advanced optoelectronic applications and sensoring

Proposer: Rita Magri

Tutor: Rita Magri

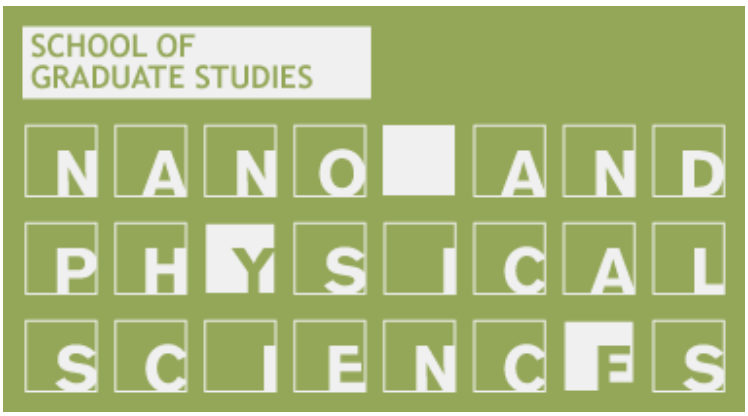
Type: (Theoretical/Experimental) Theoretical

abstract: (no more than 800 characters)
Given the very high aspect-ratio, nanowires show a huge potential for a number of applications. For instance, homogeneously doped semiconductor nanowires represent key building blocks for a variety of electronic and optoelectronic devices. Improved structural properties such as shape, length, sidewall reconstructions, and defect density of the nanowires will increase the carrier control and increase the level of sensitivity. The thesis is about the application of ab-initio and semi-empirical schemes, already developed in our group, to the study of the structural and electronic properties related to semiconductor nanowires shape and sidewalls. The aim is to determine the appropriate binding sites for small molecules and the mechanism of molecule adsorption. Finally the change of the optical and transport responses as a consequence of the molecular absorption will be investigated.

Collaborations: (other National or International groups directly involved in the research)
Prof. Lucia Sorba, NEST, Pisa (experiments)

Coworkers: (at UniMORE)
Marcello Rosini

Extra-bourse (15keuero/year) available: (yes/no)
no
support for hosting foreign students (4Keuro/year) available: (y/n)
possible for one year
supplementary information: (webpage address if available).
acmnew34.unimore.it
www.nanomodelling.unimore.it



Proposal for a PhD Thesis 2009

Title: Theoretical simulation of Single Molecule Magnets

Proposer: Valerio Bellini

Tutor: Franca Manghi

Type: Theoretical

abstract: (no more than 800 characters)
Single Molecule Magnets are a new class of zero-dimensional magnetic materials that represent the smallest possible magnetic devices, offering a controllable, bottom-up approach to nanoscale magnetism.
The goal of this PhD research project is to understand how single molecule magnets can be organized, tuned, and addressed on a surface. We will study the adsorption of a promising class of single molecule magnets on different surfaces, taking care on how these molecules orient their magnetization axes with respect to the surface, and how the molecular spins can be addressed by applying, for instance, local electric fields
We will tackle these problems on a theoretical ground realizing computational simulations. To deal with such complex systems and to describe their diverse functionalities, it will be necessary to put together the predictive power of ab-initio methods and the flexibility of model Hamiltonians approaches.

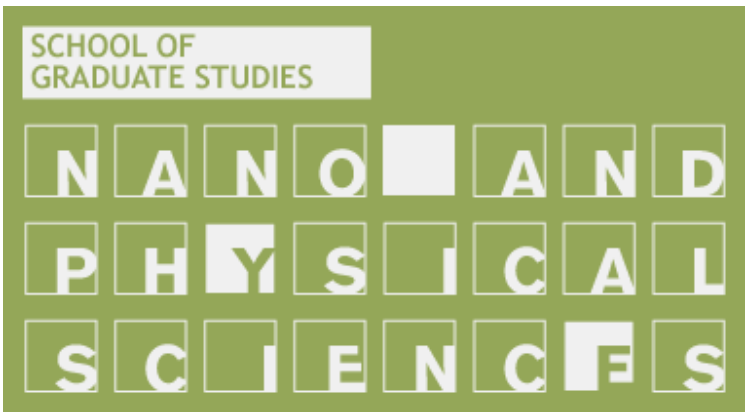
Collaborations: (other National or International groups directly involved in the research)

Coworkers: (at UniMORE)
Prof. Marco Affronte (exp), Dr. Filippo Troiani (theo)

Extra-bourse (15keuero/year) available: no

support for hosting foreign students (4Keuro/year) available: no

supplementary information: (webpage address if available)
http://www.quantumsolids.unimore.it/



Proposal for a PhD Thesis 2009

Title: Titania nanoparticles for photovoltaic

Proposer: Stefano Ossicini

Tutor: Stefano Ossicini

Type: Theoretical

abstract:
Dye- sensitized solar cells (DSSC) are a low-cost alternative to the conventional solar cells. In such devices, light is absorbed by a sensitizer (dye molecule), which is anchored to the surface of a wide band semiconductor (TiO_2). Charge separation takes place at the interface via photo-induced electron injection from the dye into the conduction band of the solid. Density functional theory (DFT) and Time-Dependent (TD) DFT calculations will be performed in order to investigate the structural, electronic, and optical properties of a set of dye-sensitized TiO_2 nanostructures. In particular we will investigate the interfacial electronic structure between the dyes and the TiO_2 surface in terms of molecular orbitals, effective density of states, estimated electronic coupling strengths, and injection times, realizing thus a realistic model that can help to understand and optimize both the structure and the electronic properties of dye-TiO2 interfaces.

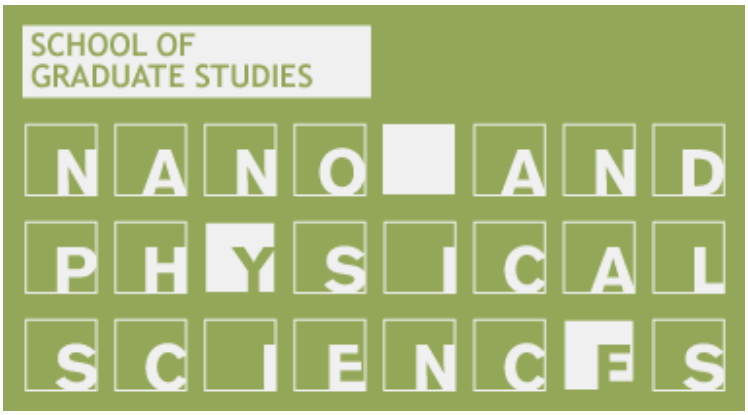
Collaborations: (other National or International groups directly involved in the research)
Prof. D. Ninno, Universita` di Napoli Federico II (Theory)
Prof. A. Rubio, Universidad del Pais Vasco (Spain) (Theory)

Coworkers: (at UniMORE)
Ivan Marri

Extra-bourse (15keuero/year) available: (yes/no)
No

support for hosting foreign students (4Keuro/year) available: (y/n)
No

supplementary information: (webpage address if available).



Proposal for a PhD Thesis 2009

Title: DOLP: Development of an optical layer for a protein chip.

Proposer:
L. Pavesi/Ossicini

Tutor:
L. Pavesi/Ossicini

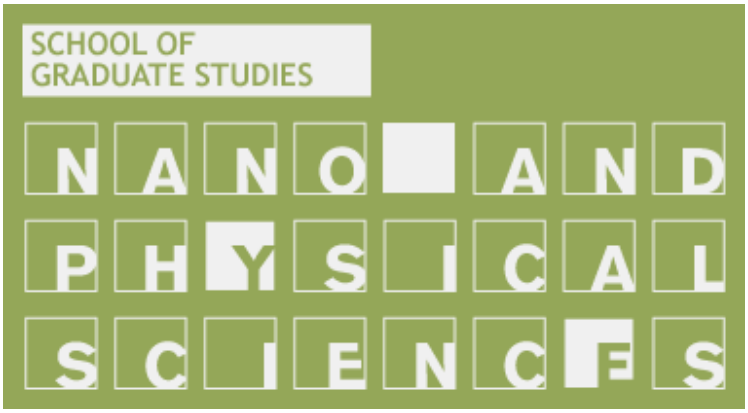
Type: (Theoretical/Experimental)
Experimental/Theoretical

abstract: (no more than 800 characters)
This project will tackle the challenge to develop an optical layer to be used in miniaturized proteins chips. Optical means are mostly used today in protein chips, this proposal aims at integrating an optical network among the many bioreactors of a protein chip. DOLP targets at the development of an optical layer through which optical signals can be channelled into and out of the protein chip. Light-matter interaction in the bioreactors will allow testing the proteins. Two main detection methods will be experimented: one which is based on labelling each protein with a cromophore and the other which is label free and is based on protein capture by ring-resonators. Both silicon based and polymer based waveguides will be tested for the optical layer. Model calculations for the system will be performed.

Collaborations: (other National or International groups directly involved in the research)
University of Trento, Nanoscience Lab
Bruno Kessler Foundation, Materials and Microsystems centre
CIVEN
CNR, Materials and Devices department

Extra-bourse (15keuero/year) available: (yes/no)
maybe

support for hosting foreign students (4Keuro/year) available: (y/n) no
supplementary information: (webpage address if available).http://naomi.science.unitn.it/
Title: Quantum effects in molecular nanomagnets.



Proposal for a PhD Thesis 2009

Title:
Graphene-based nanostructures and their interaction with magnetic systems

Proposer:
Deborah Prezzi, Prof. Elisa Molinari

Tutor:

Type: (Theoretical/Experimental)
Theoretical -- Computational

Abstract:
Graphene is being studied as a novel material with exceptional properties. While extended graphene is paramagnetic, some of its derivatives are dominated by intrinsic magnetic features. This is the case of graphene stripes and dots with specific edge termination, or defected graphene nanostructures. This thesis will focus on the coupling of such structures with magnetic molecules and/or surfaces in order to explore new routes for magnetic sensing and spintronics applications. The PhD activity will concentrate on first-principles simulations of structural, electronic, and transport properties of the systems, by means of numerical codes based on density functional theory (DFT). A treatment of electronic correlations beyond mean field may also be required, based on either ab-initio or model approaches. Part of the theoretical activity will be developed in close collaboration with national and international experimental groups.

Collaborations: (other National or International groups directly involved in the research)
Nanomagnetism Group at S3, Modena.
Nanoscale Science and Engineering Center (NSEC) & Columbia University – New York City, NY.

Coworkers: (at UniMORE)
Dr. Arrigo Calzolari, Dr. Andrea Ferretti
Extra-bourse (15keuero/year) available: (yes/no)
to be defined
support for hosting foreign students (4Keuro/year) available: (y/n)
to be defined

supplementary information: (webpage address if available).

Proposal for a PhD Thesis 2009

Title: Surface chemistry and atomistic processes at interfaces of technological interest: their effects on nanotribological properties.

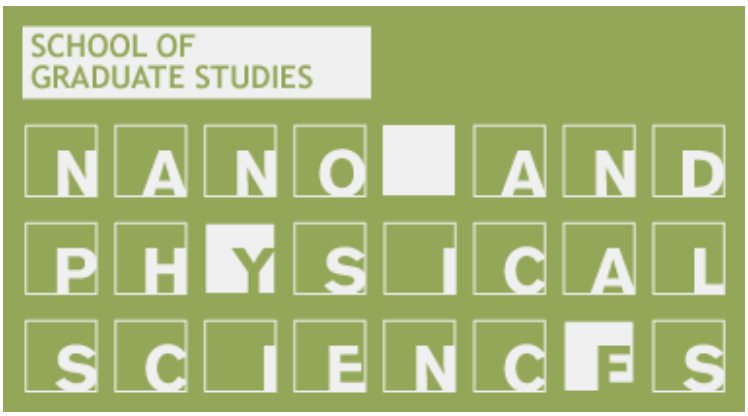
Proposer: Dr. Clelia Righi

Tutor: Prof. Elisa Molinari

Type: Theoretical

Abstract:
The dominance of surface effects at the nanoscale implies that the tribological properties of interacting materials can be critically influenced by the surface chemical composition and morphology. Carbon-based materials have tremendous potential in nanotechnology applications because of their outstanding and often unsurpassed tribological performances. Different experimental investigations highlighted the influence of the environment on the tribology of these materials. The first purpose of the present PhD project is to investigate the role of air humidity in influencing the friction and adhesion of carbon surfaces in relative motion. This will be accomplished by means of *ab initi*o simulation of the tribochemical processes occurring at sliding interfaces in presence of water molecules.
Ab initio molecular dynamics simulations, based on the Car Parrinello method, will be used also to investigate the tribochemical reactions occurring at another class of systems of technological interest: P- or S-based additives at iron interfaces. These systems are of great interest for ordinary automotive applications. Investigating the chemical reactions occurring in lubricant additives under tribological stress is essential to understand their antiwear functionality and to design improved, environment-friend additives.

Collaborations:
Dr. Olivier Lerasle,
TOTAL - Solaize Research Center,
Lubricant department – Strategic Research and Base Oils
Coworkers: (at UniMORE)
Gruppo sperimentale di Sup&rman, Dr. Alberto Rota
Extra-bourse (15keuero/year) available: (yes/no)
no
support for hosting foreign students (4Keuro/year) available: (y/n)
no
supplementary information: (webpage address if available).



Proposal for a PhD Thesis 2009

Title: Atomic scale friction and adhesion of silicon carbide, silicon, and diamond

Proposer: Dr. Clelia Righi, Prof. Mauro Ferrario

Tutor: Prof. Mauro Ferrario

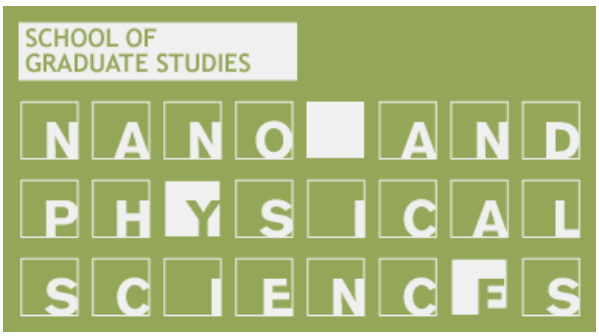
Type: Theoretical

abstract:
Because of its high Young's modulus, SiC, has many outstanding mechanical properties, such as very low coefficient of friction, high hardness, and high wear resistance, which allow for the application of SiC as hard surface coating. Coating surfaces are usually rough, and friction is generated between surface asperities where the contact area is on the atomic scale. The single asperity contact is reproduced by means of experiments based on a tip scanning the surface. At the same level, atomistic simulations can be employed to provide insight into the behavior within these contacts. While few theoretical investigations of the tribological properties of diamond exist, analogous comprehensive studies on silicon-based materials are yet lacking.
The purpose of the present PhD project is to investigate surface effects such as the surface chemical composition, its orientation and reconstruction, on the friction and adhesion properties at the nanoscale. The tribological behavior of SiC will be considered and compared with that of diamond and of silicon. This will be accomplished by means of ab initio molecular dynamics (MD) eventually combined with classical MD simulations relaying on realistic potential able to reproduce the chemical behavior of the materials in contact.

Collaborations: gruppo sperimentale di Sup&rman: Dr Alberto Rota

Coworkers: (at UniMORE): Prof. C. M. Bertoni

Extra-bourse (15k euro/year) available: (yes/no)
no
support for hosting foreign students (4Keuro/year) available: (y/n)
no
supplementary information: (webpage address if available).



Proposal for a PhD Thesis 2009

Title: control of friction at the nanoscale

Proposer: Alberto Rota**,** Sergio Valeri

Tutor: Sergio Valeri

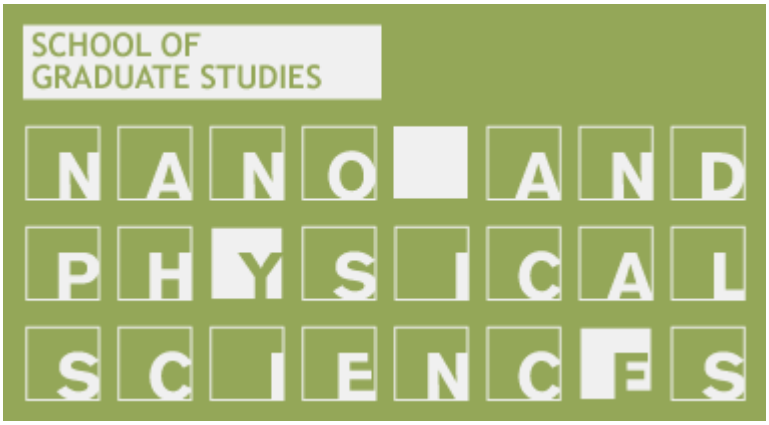
Type: Experimental

abstract: Understanding the complex tribological processes occurring at the interface of materials is central to pure and applied sciences as well as to many technological problems, including friction, adhesion, lubrication, wear, contact formation. In particular the comprehension and control of friction processes at the nanoscale represents an important challenge both for experimental and theoretical research. This is related to the fact that at the nanoscale surface forces often exceed volume forces and adhesion becomes an important parameter in the sliding processes. Also, adhesive forces are strongly influenced by contaminants at the surface, including adsorbed water molecules related to air humidity.
The proposed research activities will comprise experimental investigations of different approaches to control friction at the micro-nano scales. Specific objectives are as follows.
Patterned surfaces: experimental study of dry and lubricated contacts on micro- and nano- patterned surfaces to control and improve mechanical and tribological performances of hi-tech devices. Theoretical/numerical investigation and experimental development of optimized efficient geometries and wide-area fabrication of nano-patterned surfaces.
Mechanical control of friction: modeling feedback and direct methods of controlling frictional forces through the application of external oscillatory perturbations in the stick-slip and sliding regimes of motion. Experimental characterization of changes in contact area and frictional resistance induced by normal and lateral vibration of nano-contacts, nano-contact arrays, and large spatially extended systems.

Collaborations: (other National or International groups directly involved in the research)
- M. Urbakh, School of Chemistry, Tel Aviv University, Tel Aviv, Israel.
- E. Meyer and E. Gnecco, Institute of Physics, University of Basel, Switzerland.

Coworkers: (at UniMORE)
Theoretical Group: Dr. M. Clelia Righi

Extra-bourse (15keuero/year) available: no
support for hosting foreign students (4Keuro/year) available: yes
supplementary information: (webpage address if available).
See the activity line : tribology and coatings at the website: http://www.s3.infm.it/line3_index.html
The proposed PhD activity will be performed in strict connection with the technological activities on nanomechanics at the SUP&RMAN laboratory (http://suprman.cineca.it/)



Proposal for a PhD Thesis 2008

Title: *Ab initio* study of nonlinear optical properties in molecules and crystalline solids

Proposer: Carlo Andrea Rozzi

Tutor: Franca Manghi

Type: Theoretical

Abstract: The accurate theoretical description of optical properties of matter is a crucial step in the project of solid state optoelectronic devices. A compelling problem is how to protect a component from overillumination by limiting its absorption coefficient for high intensity incident field. In state-of-art technology the usual active limiting techniques are not always appropriate solutions, since the systems may be subject to picosecond light pulses. Passive devices, on the other hand, may display an ultrafast non linear response. The *ab initio* theoretical description of this process must rely on a theory capable of both resolving in time the electron dynamics of the system, and describing the optical response in the non linear regime. This thesis is devoted to the application of Time Dependent Density-Functional Theory to this topic, with particular regards to the differences in the treatment of polarization in finite and infinite periodic systems.

Collaborations:

- Xavier Andrade, Dpto. de Física de Materiales, Universidad del País Vasco, San Sebastián
- Angel Rubio, Dpto. de Física de Materiales, Universidad del País Vasco, San Sebastián
- Luigi Sangaletti, Università Cattolica del Sacro Cuore, sede di Brescia

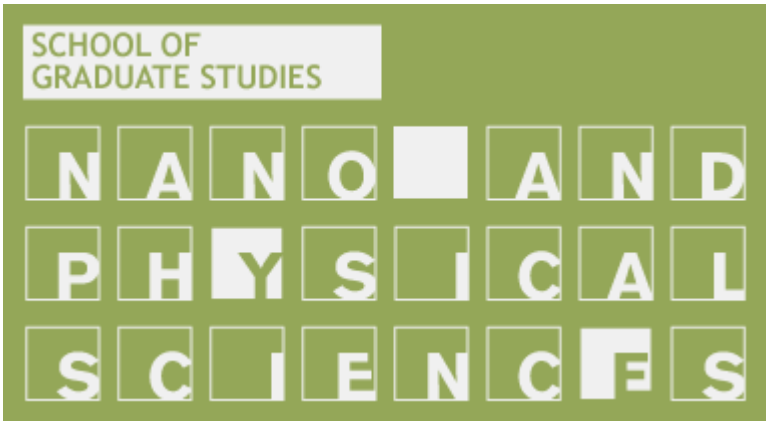
Coworkers: Daniele Varsano, INFM-CNR S3, Modena

Extra-bourse (15keuero/year) available: no

support for hosting foreign students (4Keuro/year) available: no

supplementary information: (webpage address if available):

- T. R. Oliveira *et al*., Appl. Phys. Lett. 89, 211912 (2006)



Proposal for a PhD Thesis 2008

Title: Development of time-dependent theory for photoemission spectroscopy

Proposer: Carlo Andrea Rozzi

Tutor: Franca Manghi

Type: Theoretical

Abstract: Time resolved (femtosecond) photo electron spectroscopy is a powerful technique for the characterization of nanoscale and biological systems. Unfortunately perturbation theory based techniques are only able to accurately describe the one-electron removal spectra within the regime of weak incident field, while beyond an irradiance of the order of 10^{12} Wm^{-2}, the complexity of the full many-body solution of the problem is such that already a system with more than two electrons turns out to be untractable. Time dependent Density-Functional theory is the ideal tool to be developed in the description of this spectroscopy, since it merges the computational advantage of DFT when dealing with many electrons systems, and the flexibility of a beyond ground-state approachin which weak and intense field ranges can be faced on the same footing.

Collaborations:

- Eberhard K. U. Gross, Institut für Theoretische Physik, Freie Universität Berlin, Berlin
- Angel Rubio, Dpto. de Física de Materiales, Universidad del País Vasco, San Sebastián

Coworkers: Daniele Varsano, INFM-CNR S3, Modena

Extra-bourse (15keuero/year) available: no

support for hosting foreign students (4Keuro/year) available: no

supplementary information: (webpage address if available):

- A. Pohl *et al.*, Phys. Rev. Lett. 84, 5090 (2000)
- D. Varsano, PhD thesis, Universidad del País Vasco, San Sebastián, 2006

SCHOOL OF GRADUATE STUDIES

NANO AND PHYSICAL SCIENCES

Proposal for a PhD Thesis 2008

Title: Time resolved analysis of charge transfer in light harvesting organic molecules

Proposer: Carlo Andrea Rozzi

Tutor: Franca Manghi

Type: Theoretical

Abstract: This proposal is devoted to the study of attosecond time resolved electron dynamics in organic molecules and supamolecular assemblies of interest for photovoltaic applications. After a photoinduced excitation these systems are able to efficently separate electrons and holes effectively acting as elementary units for solar energy conversion. A crucial step in achieving an high efficient device consists in controlling the time life of the charge separated state and minimizing the recombination probability. Time dependent Density-Functional theory will be employed to obtain a useful insight of this ultrafast dynamics, and the optical response of the system will be studied both in the linear response regime, and after ultrashort monochromatic (or suitably shaped) laser pulses.

Collaborations:

- Angel Rubio, Dpto. de Física de Materiales, Universidad del País Vasco, San Sebastián

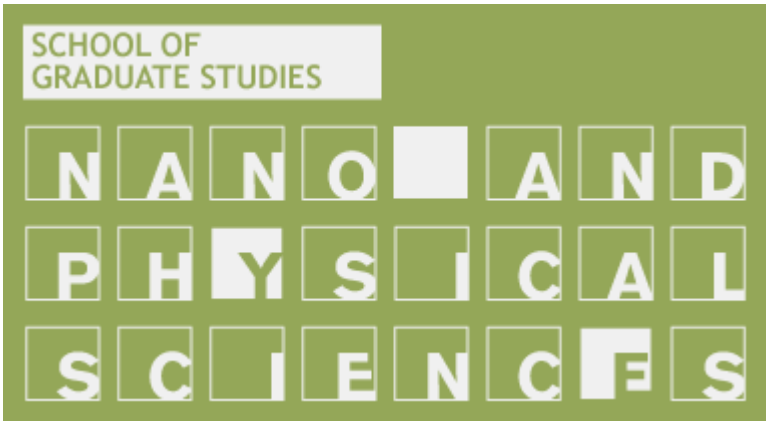
Coworkers: N. Spallanzani, Daniele Varsano, INFM-CNR S3, Modena

Extra-bourse (15keuero/year) available: no

support for hosting foreign students (4Keuro/year) available: no

supplementary information: (webpage address if available):

- P. V. Kamat, J. Phys. Chem. C 111, 2834 (2007)
- N. Spallanzani *et al.*, submitted to Nanoletters



Proposal for a PhD Thesis 2008

Title: Time dependent study of 1D and 2D quantum dots array

Proposer: Carlo Andrea Rozzi

Tutor: Franca Manghi

Type: Theoretical

Abstract: The state-of-art techniques for nanofabrications allow nowadays to build semiconductors arrangements of quantum dots, namely arrays of confined electron islands. These low dimensional nano systems often display unespected properties, with respect to their 3D counterparts. In particular 1D and 2D arrays of quantum dots are an ideal case study for the investigation of the interplay between electronic and magnetic properties of artificial atoms in periodic arrangements. This thesis is particularly devoted to the study of the cross effects of periodic order and dimensionality on these nanosystems. Both the ground state and the excited state properties can be investigated by means of Time dependent Density-Functional Thory, which can be applied to the description of ultrafast electron dynamics.

Collaborations:

- Esa Räsänen, Nanoscience Center, Department of Physics, University of Jyväskylä, Finland
- Alberto Castro, Institut für Theoretische Physik, Freie Universität Berlin, Berlin

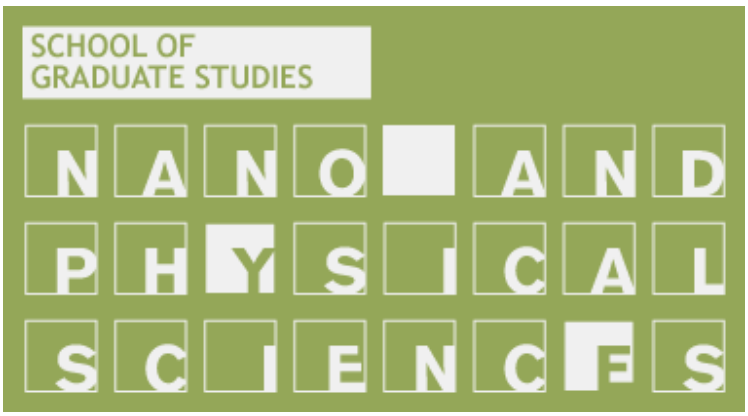
Coworkers: Daniele Varsano, INFM-CNR S3, Modena

Extra-bourse (15keuero/year) available: no

support for hosting foreign students (4Keuro/year) available: no

supplementary information: (webpage address if available):

- M. Koskinen *et al.*, Phys. Rev. Lett. 90, 66802 (2003)
- C. A. Rozzi *et al.*, Phys. Rev. B 73, 205119, (2006)



Proposal for a PhD Thesis 2009

Title: Quantum-information processing with molecular nanomagnets

Proposer: Filippo Troiani (CNR-INFM "S3")

Tutor: Filippo Troiani (CNR-INFM "S3"),
Marco Affronte (CNR-INFM "S3" and University of Modena and Reggio Emilia)

Type: Theoretical

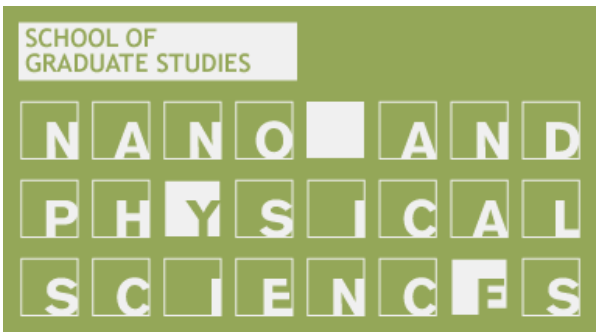
Abstract: In the last years, antiferromagnetic spin clusters have been recognized as a promising class of candidate qubits. Relevant to this aim are the possibility of synthetizing arrays of identical units, and the flexibility with which both the effective spin-spin interactions and the environmental couplings can be tailored by coordination chemistry. The aim of the present project is that of theoretically addressing at least one of the key issues in the implementation of quantum-information processing with metallic molecular antiferromagnets. These include: (i) electron-spin decoherence due to hyperfine interactions: dynamics of electron-nuclear entanglement; strategies for controlling decoherence; (ii) electrical manipulation of the molecular spin; (iii) controlled generation, characterization and decoherence of entangled states in coupled molecular antiferromagnets.

Collaborations: D. Loss (Univ. of Basel, Switzerland), G. Amoretti (Univ. of Parma), R. Winpenny (Univ. of Manchester).

Coworkers: V. Bellini.

Extra-bourse (15keuero/year) available: to be defined.

Support for hosting foreign students (4Keuro/year) available: to be defined.
Supplementary information: http://www.nanoscience.unimore.it/filippo.html



Proposal for a PhD Thesis 2009

Title: Mechanical properties and phenomena at the nanoscale

Proposer: Sergio Valeri

Tutor: Sergio Valeri

Type: Experimental

abstract: Understanding how materials deform and fail at the nanoscale is a tremendous challenge for basic research. Moreover, with increasing device miniaturization in nanotechnology, mechanical issues impose increasingly serious constraints and limitations on the performance and lifetime of advanced technological microdevices (such as Micro and Nano Electro-Mechanical Systems, MEMS and NEMS) This proposal deals with experimental study of the mechanical properties, plastic deformations and fracture mechanisms of thin and ultra-thin films, nano-objects (nano-pillars with variable shape and geometry), and one-dimensional structures (nanotubes, nanowires and nanofibers), with the help of a dedicated Atomic Force Microscope (AFM) used as a nanoindenter device. Study and improvement of the AFM indentation technique, developing new indentation devices (new geometries for the AFM probes). Study of the substrate-indenter interaction (flow-stress and dislocations mobility) through an in-situ TEM-indentation system. Substrate elastic properties and dissipative behavior of the tip-surface interaction addressed by AFM in dynamic mode.

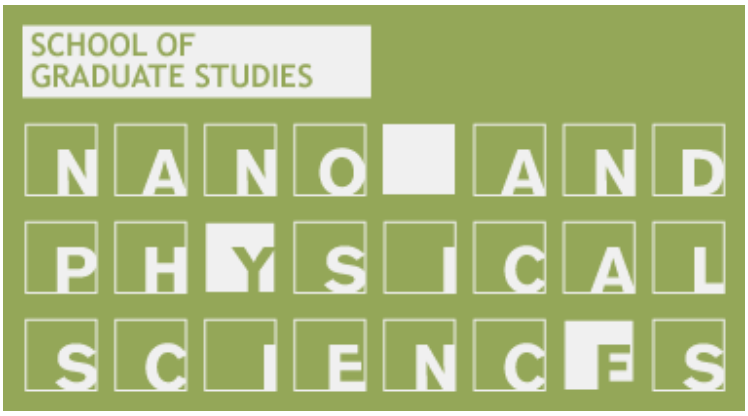
Collaborations: (other National or International groups directly involved in the research)
- N.M. Pugno, Department of Structural Engineering, Politecnico di Torino, Italy.
- U. Valbusa and R. Buzio, Physics Department, University of Genova, Italy.
- R.S. Ruoff, Mechanical Engineering Department, University of texas at Austin, USA.

Coworkers: (at UniMORE)
- G.C. Gazzadi, CNR-INFM-S3; - S. Frabboni, CNR-INFM-S3; - S. Zapperi, CNR-INFM-S3

Extra-bourse (15keuero/year) available: no

support for hosting foreign students (4Keuro/year) available: yes

supplementary information: (webpage address if available).
See the activity line : tribology and coatings at the website: http://www.s3.infm.it/line3_index.html
The proposed PhD activity will be performed in strict connection with the technological activities on nanomechanics at the SUP&RMAN laboratory (http://suprman.cineca.it/)



Proposal for a PhD Thesis 2009

Title: Few-electron states in carbon-based nanostructures

Proposer:
Massimo Rontani

Tutor:
Elisa Molinari

Type: (Theoretical/Experimental)
Theoretical

abstract: (no more than 800 characters)
The investigation of carbon-based nanostructures is a hot topic for novel fields such as spintronics and quantum information science. A major challenge is the understanding of fundamental properties of few-electron complexes in systems such as carbon-nanotube quantum dots and graphene flakes. In fact, this study is made difficult by the unique features of the underlying material, which exalt the role of interaction among electrons. This high-risk high-gain Thesis takes care in full of electron correlation, by applying the exact diagonalization method to realistic model Hamiltonians. The final goal of the research is the prediction of observable properties connected to electron spectroscopies, therefore comparison with experimental data will be explicitly sought.

Collaborations: (other National or International groups directly involved in the research)
S. M. Reimann (University of Lund, Sweden), L. J. Sham (University of California San Diego, California)
Coworkers: (at UniMORE)
Arrigo Calzolari, Deborah Prezzi, Carlo Cavazzoni
Extra-bourse (15keuero/year) available: (yes/no)
no
support for hosting foreign students (4Keuro/year) available: (y/n)
no
supplementary information: (webpage address if available).
www.nanoscience.unimore.it/max.html