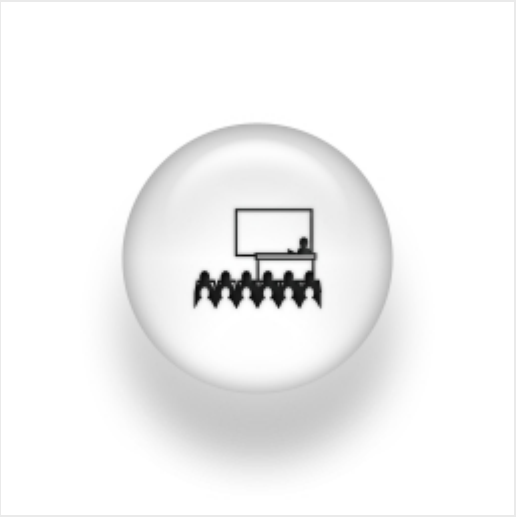
Sculpting Membranes. Mechanisms of Curvature Generation by Proteins

Tuesday, 16 December 2008, 15:00-16.00

Dr. Felix Campello



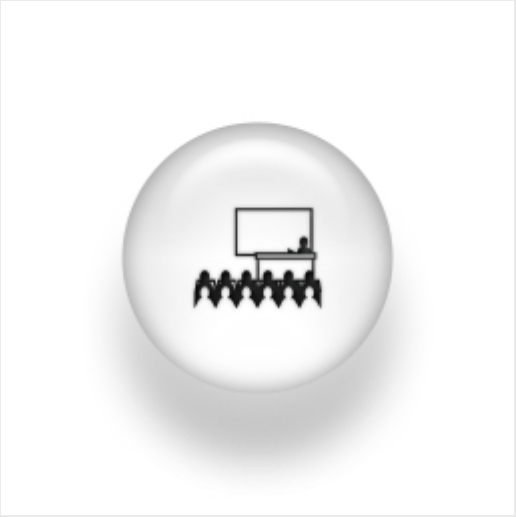
Dept. Estructura i Constituents de la Materia, Facultat de Fisica, Universitat de Barcelona

A wide spectrum of intracellular processes is dependent on the ability of cells to dynamically regulate membrane shape. Membrane bending by proteins is necessary for the generation of intracellular transport carriers and for the maintenance of otherwise intrinsically unstable regions of high membrane curvature in cell organelles. Understanding the mechanisms by which proteins curve membranes is therefore of primary importance. Crescent shaped N-BAR domains containing amphipathic helices can induce membrane curvature by two mechanisms: the scaffolding mechanism due to the very shape of the BAR dimer, and the hydrophobic insertion mechanism by which small shallow inclusions penetrate the membrane matrix and act as a wedge changing the local membrane curvature. In this seminar, we will focus on this latter mechanism, and study it from a quantitative point of view. We use an elastic model of the lipid bilayer, taking into account the internal strains and stresses generated by the presence of an inclusion. We show that large membrane curvatures found in in vitro experiments can be ascribed to this mechanism.

Excitons in Carbon based quasi-1D systems: an ab-initio study of nanotubes and graphene ribbons

Wednesday, 10 December 2008, 12:00-13.00

Dr. Deborah Prezzi

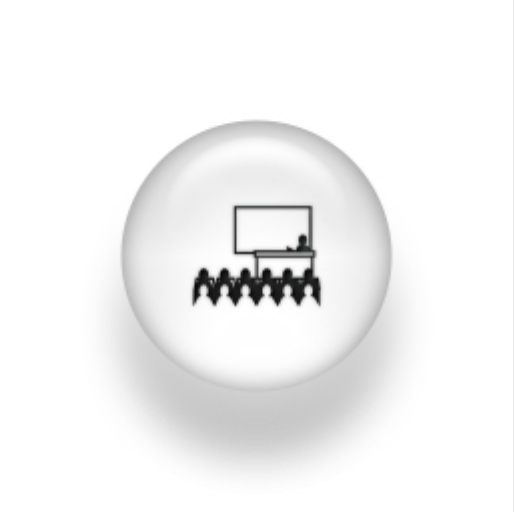


Physics Dept, University of Modena, and Natl Center S3 of INFM-CNR, Modena, Italy

We discuss the main characteristics of optical excitations in C semiconductor nanotubes and nanoribbons, as obtained from ab-initio many-body calculations. Our theoretical approach includes both self-energy corrections and excitonic effects through the GW-BSE formalism, providing full understanding of excited-state properties.
Electron-hole interaction is found to suppress the van Hove singularities -as known for other 1D systems- and introduces strongly bound excitonic peaks.
For C nanotubes, we show that exciton binding energy must thus be extracted from two-photon optical spectra and is of the order of several tenths of eV. A complete symmetry analysis of the excitonic states allows to understand the luminescence features observed in experiments [1]. In graphene ribbons we analyse different geometries and show that strong exciton binding is accompanied by relevant effects of the ribbon termination [2]. Based on simple prototype structures, we also discuss the possibility to obtain strong 0D confinement in graphene dots and antidots [3].
[1] Maultzsch et al., Phys. Rev. B 72, 241402(R) (2005) [2] D. Prezzi et al., arXiv:0706.0916v1 (2007) [3] D. Prezzi et al., in preparation (2007).

Electrical conduction through molecules: Influence of endgroups and sidegroups

Wednesday, 3 December 2008, 12:00-13.00

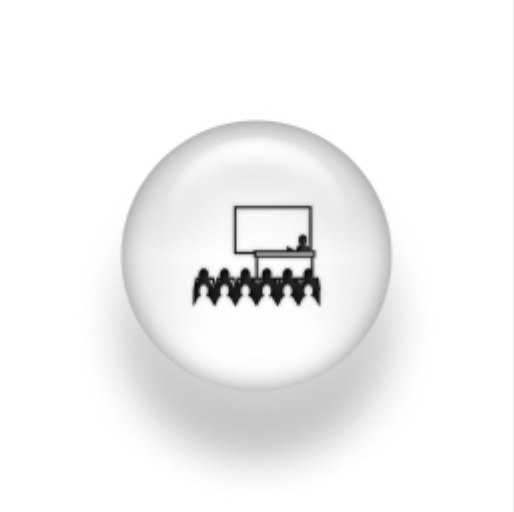


Dr. Artur Erbe
Universitaet Konstanz, Germany

Molecular electronics aims for scaling down electronics to its ultimate limits by choosing single molecules as the building blocks of active devices. The advantages of this approach are the high reproducibility of molecular synthesis on the nanometer scale, the ability of molecules to form large structures by self-assembly and the huge versatility of molecular complexes. On the other hand, conventional contacting techniques cannot form contacts on the single molecule scale and imaging techniques nowadays cannot provide a detailed image of such junctions. Therefore the fabrication has to rely on some degree of self-organization of the constituents and the proof that a molecule has been contacted successfully can be only given by indirect methods, for example by measuring the current transport through the junctions.
In this talk the role of the molecular functionalities which link the molecule to the metallic electrodes will be investigated. We studied a series of simple molecules, equipped with varying linking groups, using the mechanically controlled break junction technique and compared the conduction properties.
In addition, a simple toy molecule is presented in order to understand the molecular transport and compared to the measured data. A more complex molecule showing a pronounced switching effect upon changes of the applied bias voltage is shown to demonstrate the possibility of functional molecular electronic building blocks. DNA molecules are ideal candidates for self-organizing electrical circuits. Our measurements on G-quadruplex oligonucleotides reveal reproducible conduction behavior which sustains stretching of the molecular junctions.

Magnetotransport in non-magnetic inhomogeneous media

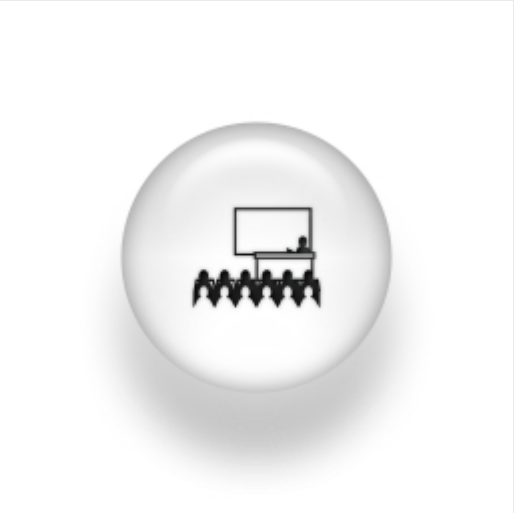
Wednesday, 26 November 2008, 12:00-13.00



Dr. Meera Parish
Princeton Center for Theoretical Science Princeton University
When the transport properties of a material change substantially in a magnetic field, it is often due to some kind of magnetic order. In particular, if the dielectric function is strongly magnetic-field-dependent, it is usually ascribed to coupled magnetic and elastic order, such as is found in the multiferroics. However, here I will show that magnetism is not necessary to produce either a magnetoresistance or a magnetocapacitance when the material is inhomogeneous. By considering a two-dimensional, composite medium, I find a characteristic dielectric resonance that depends on magnetic field. I propose this as a possible signature of inhomogeneities and I argue that this behavior has already been observed in materials such as nanoporous silicon.

Cluster-based density functional approach to transport through molecular and atomic contacts

Thursday, 20 November 2008. 15:00-16.00



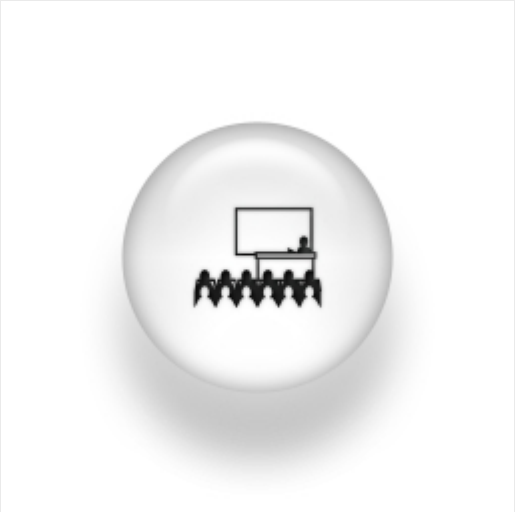
Dr. Fabian Pauly

Universidad de Karlsruhe (Alemania)

We present our recently developed ab-initio method to model quantum transport in atomic and molecular contacts. The electronic structure is treated at the level of density functional theory, and the parameters needed to describe transport are extracted from finite clusters. As applications, we study (i) the tilt-angle and temperature-dependent conductance of biphenyl-derived molecules, (ii) the length-dependent conductance and thermopower of oligophenylenes, and (iii) highly conductive junctions of benzene coupled directly to Pt electrodes. If time permits, we will also present recent more qualitative work on the influence of light on the current in molecular junctions.

Tunable superfluids in ultracold atomic gases

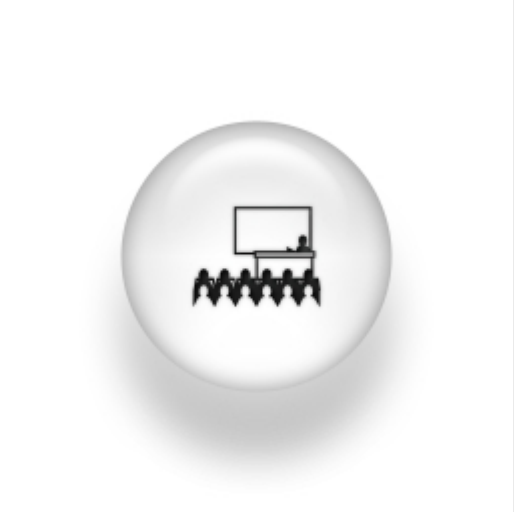
Wednesday, 12 November 2008, 12:00-13.00



Dr. Francesca Maria Marchetti
Departamento de Fisica Teorica de la Materia Condensada (UAM)
Thanks to the recent experimental advances, ultra-cold atomic gases now provide the ultimate playground in which to realise and study a large variety of condensed matter phenomena. In particular, the ability to manipulate and control ultra-cold atomic gases provides a unique experimental system in which to explore pairing phenomena and superfluidity. Following the successful realisation of the crossover from the BCS state of Cooper pairs to the Bose Einstein condensation of diatomic molecules, attention has turned to the consideration of more exotic superfluids. A subject that has attracted particular theoretical and experimental interest is that of Fermi condensates with imbalanced spin populations, owing to the potential relevance of polarised Fermi condensates to QCD and magnetised superconductors. Even richer scenarios are expected for heteronuclear resonances in Bose-Fermi mixtures. I will discuss the work I have carried on both subjects and the relevance of our findings to recent experiments.

Molecular simulations in the Era of GPUs

Friday, 31 October 2008, 12:00-13.00

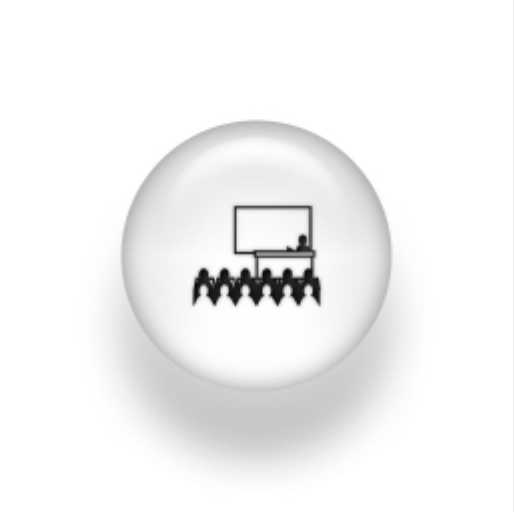


Dr. Gianni De Fabritiis
Universidad Pompeu Fabra (UPF)

The recent introduction of cost-effective accelerator processors (APs), such as the IBM Cell processor and Nvidia's graphics processing units (GPUs) represents an important technological innovation for computational science. Present accelerator processors can deliver over an order of magnitude more floating-point operations per second (flops) than standard processors, broadly equivalent to a decade of Moore's law growth. In conjunction with distributed and grid computing solutions these devices can be deployed to become a new form of supercomputing as in PS3GRID.net and GPUGRID.net, where accelerated molecular simulations are used to simulate hundreds of protein-ligand complexes with full molecular specificity, a crucial requirement of in silico drug discovery workflows.

Exciton and Polariton Manipulation Within Semiconductor Microstructures

Monday, 23 June 2008, 15:00-16.00



Dr. Frank Bello
University of Sheffield, U.K.
A review is presented of the theoretical/modelling constructs as well as experimental techniques used in order to qualitatively and quantitatively describe the dynamics of the exciton and polariton within semiconductor microcavities containing an embedded quantum dot. Subsequent effects such as antibunching, controlled rotations (CROT), as well as the optical parametric amplifier (OPO) are studied. For antibunching effects we look at various pumping techniques of the system and how this will inhibit or promote single photon emission with a full quantization treatment of the field. Also within full field quantization, the spectrum of the OPO is theoretically derived and modelled to include scattering effects between all the modes of the amplifier.

Toward molecule-machines at the nanoscale

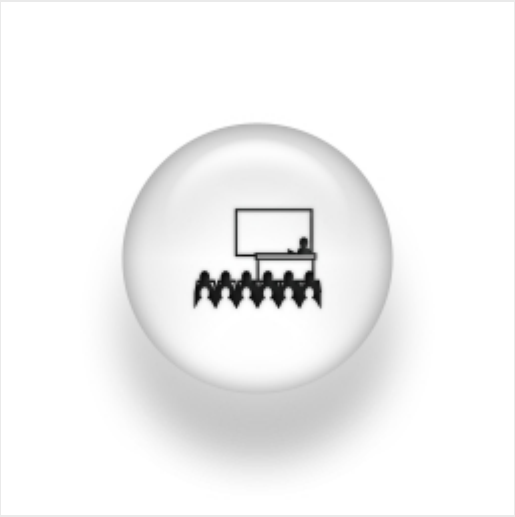
Monday, 16 June 2008, 15:00-16.00

Dr. C. Joachim
The Nanoscience Group, CEMES-CNRS, 29, Rue J. Marvig, BP 94347, 31055 Toulouse Cedex, France and A*STAR VIP Atom Technology, IMRE, 3 research Link, Singapore

There is no physical limitation for the miniaturization of a machine down to the scale of a single molecule or conversely, to monumentalize a molecule until it becomes a machine. A few prototypes of mechanical molecule-machine are already under testing like the molecule-wheelbarrow or the molecule-atom cleaner, a few others molecules have been designed and used as experimental nano-devices like a molecule-gear or the series of the Lander molecules to study an atomically clean electronic contact to a metallic pad. Other molecules are at their early design and synthesis stages like a motor- molecule-motor, a molecule equipped with four wheels or molecule-logic gates like a molecule-semi-classical OR gate or a molecule-quantum ½ digital adder.
Those examples will be illustrated because (1) they are also driving new challenges in the modeling of the behavior of a large molecule on a surface and (2) they are driving new instrumentation developments to exchange data, orders, synchronization signals or energy with a single (and always the same) molecule, just a nanometer in size.

Weak localization-like processes in gapped systems in connection with the realization of a source of entangled pairs of electrons

Monday, 26 November 2007, 12:00-13.00



Dr. Regis Melin
Low temperature Physics Laboratory. CNRS, Grenoble
A lot of interest is devoted to realize experimentally devices in which pairs from a superconductor are splitted in two different normal or ferromagnetic electrodes, therefore realizing a source of entangled pairs of electrons.
After reviewing some experiments, I will discuss higher order processes in the tunnel amplitudes already for a normal metal – insulator – normal metal junction. Then going to normal metal – superconductor – normal metal junctions, I will show that the non local conductance contains two terms of opposite sign: i) a term corresponding to a double Andreev process, and ii) weak localization-like tunneling. I will also discuss a simple model for multiple reflections on disorder in the normal electrodes, or on the

sample boundaries. Finally, I will discuss the same weak localization-like processes in experiments showing magnetoresistance oscillations in another gapped system (charge density waves pierced by nanoholes).