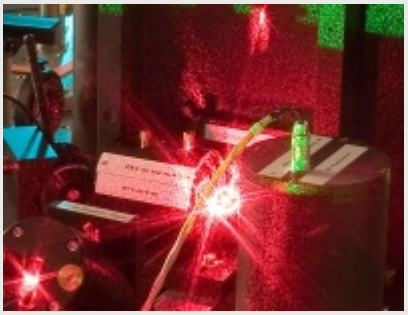
Digital Quantum Simulation with Rydberg Atoms and Ions

Wednesday, 9th May 2012. 12:00-13:00



Digital Quantum Simulation with Rydberg Atoms and Ions

Markus Müller
Departamento de Física Teórica, Universidad Complutense de Madrid

ABSTRACT:
A universal quantum simulator is a controlled quantum device that faithfully reproduces the dynamics of any other many-particle quantum system with short-range interactions. This dynamics can refer to both coherent Hamiltonian and dissipative open-system time evolution. In our talk we present a scheme, where laser-excited Rydberg atoms in optical lattices provide an efficient implementation of such a universal digital quantum simulator. After a short introduction to some basic concepts of quantum simulation and atomic Rydberg physics, we discuss how the proposed simulation architecture allows one to realize coherent Hamiltonian as well as dissipative open-system time evolution of spin models involving n-body interactions, such as e.g. Kitaev's toric code and more complex lattice gauge theories. Our simulator relies on a combination of multi-atom Rydberg gates and optical pumping to implement coherent operations and dissipative processes. We also report on recent experiments with trapped ions, which have demonstrated these concepts and the building blocks of such an open-system quantum simulator in the laboratory.

Magnetic ground states in transition-metal oxides driven by superexchange interactions

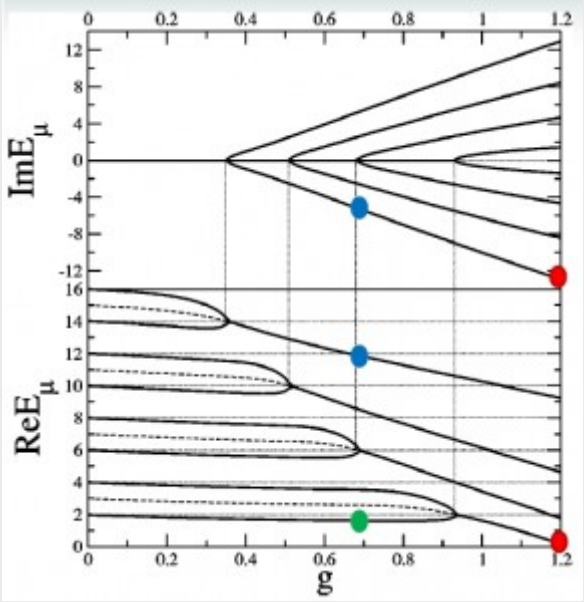
Wednesday, 25th April 2012. 12:00-13:00

Sergio di Matteo
Université de Rennes 1, France
ABSTRACT:
The aim of the present seminar is to provide a general introduction on the possible effects of superexchange interactions on magnetic ground states in transition-metal oxides. Three examples are introduced and discussed in some details: a) the case of spinel $MgTi_2O_4$; b) the case of spinel ZnV_2O_4; c) the case of Cr-doped TiO_2. The first two cases are a useful example to compare the differences in the magnetic ground states of two isostructural compounds characterized by a different filling. At the same time, case a) is also extremely pedagogical in clarifying the origin of magnetoelastic forces determined by exchange and superexchange interactions. Interestingly, in this case an exact solution of the superexchange Hamiltonian on the whole lattice can be found, leading to the formation of a so-called non-resonating valence-bond crystal. Case c), finally, is more complex to discuss, but it is introduced because nowadays the search for ferromagnetism in transition-metal doped compounds is very on fashion and the results obtained here are particularly interesting as a possible explanation for a global ferromagnetic coupling in the Cr-doped TiO_2 cell.

Integrable Richardson-Gaudin models in mesoscopic physics

Wednesday, 18th April 2012. 12:00-13:00

Jorge Dukelsky

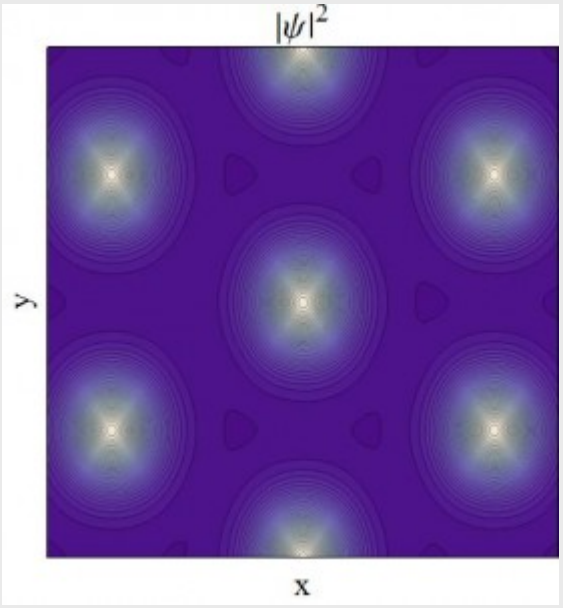


Instituto de Estructura de la Materia, CSIC

ABSTRACT:
The exact solution of the BCS Hamiltonian with non-degenerate single particle orbits was introduced by Richardson in the early sixties. Although it passed almost unnoticed, it was recovered in the last decade in an effort to describe the disappearance of superconductivity in ultrasmall superconducting grains. Since then it has been extended to several families of integrable pairing models, the Richardson-Gaudin models. However, only the rational family has been widely applied to mesoscopic systems where finite size effects play an important role. Even in the thermodynamic limit, the exact many-body wavefunction provides a unique view to the Cooper pair structure in the BCS-BEC crossover.
Two complementary implementations of the hyperbolic Richardson-Gaudin family have been recently found in condensed matter and nuclear physics. The first implementation gives rise to a p-wave pairing describing a gas of spinless fermions in a 2D lattice with $p_x + i p_y$ pairing symmetry. Using this new tool we study the quantum phase diagram which unlike the case of s-wave pairing displays a third order quantum phase transition. We make use of the exact solution to characterize the quantum phase transition and the properties of the weak and strong paring phases. The exact wavefunction of the p-wave pairing Hamiltonian gives a beautiful insight into the nature of the quantum phase transition. Moreover, it suggests the existence of an experimentally accessible characteristic length scale, associated with the size of the Cooper pairs, that diverges at the transition point. The second implementation leads to a separable pairing Hamiltonian with two free parameters that can be adjusted to give an excellent reproduction of the superfluid properties of heavy nuclei. As such it might be useful to treat other mesoscopic systems like superconducting grains or quantum dots.

Non-Abelian gauge fields in twisted bilayer graphene

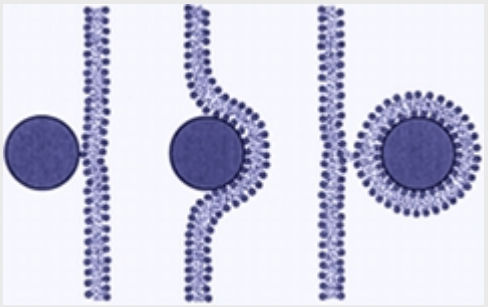
Wednesday, 11th April 2012. 12:00-13:00



Pablo San Jose
Instituto de Estructura de la Materia, CSIC, Madrid
ABSTRACT:
We present an overview of the modeling of low energy twisted graphene bilayers and of its unusual electronic properties. These include charge confinement around zero energy and velocity suppression at recurrent special twist angles. We show that these come as a consequence of non-Abelian gauge fields that arise from the spatial Moiré pattern in interlayer couplings.

Dynamical Simulations of Virus Wrapping and Budding

Wednesday, 28th March 2012. 12:00-13:00



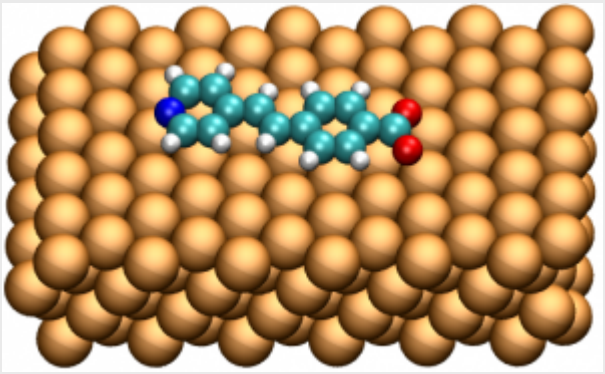
Teresa Ruiz Herrero
Departamento de Física Teórica de la Materia Condensada, UAM
ABSTRACT:
Enveloped viruses bud through the cell membrane as the final step in their replication process. For many enveloped viruses, a nucleo-protein capsid first assembles in the

cytoplasm, attaches to the membrane, and then buds.
We explore this process through modeling the wrapping of a spherical particle by a model bilayer membrane, using coarse-grained molecular dynamics simulations and a theoretical elastic model. Specifically, we study the kinetics and morphologies of wrapping as a function of the relevant system parameters, including the particle radius, the strength of the membrane-particle interaction, and the membrane bending rigidity. The theoretical model predicts a phase diagram as a function of the system parameters, which is compared to results of the dynamics simulations.
Furthermore, the simulations elucidate the dynamical mechanisms by which budding occurs and the structures of intermediate configurations.

DFT analysis of combined 3D NC-AFM and STM imaging of the Cu(100)-O oxide surface

Wednesday, 21th March 2012. 12:00-13:00

Milica Todorović



Departamento de Física Teórica de la Materia Condensada, UAM
ABSTRACT:
Investigation of novel catalytically active surfaces requires a comprehensive experimental method for the identification and rapid characterization of prospective catalytically active sites. In a bid towards functional imaging, three-dimensional atomic force microscopy (3D-AFM) in non-contact mode [1] has been combined with scanning tunnelling microscopy (STM) to study the oxygen-terminated copper (100) surface. Complex 3D data sets, obtained by simultaneously recording the tunnelling current and the AFM frequency shift, allow for site-specific quantification of forces and tunneling currents. The wealth of information obtained is remarkable, but the interpretation of the wide range of contrast modes requires a thorough characterisation of the sources of contrast in AFM and STM imaging.
We combined DFT total-energy calculations with Non-Equilibrium Green's Function (NEGF) methods for electronic transport to determine the tip-surface interaction and tunnelling current [2, 3, 4] for a large set of tip models in order to clarify the different contrast modes obtained in the experiments. We studied the features of a stable Cu(100)(2√2x√2)R45deg-O surface reconstruction and identified prospective reaction sites, before introducing model AFM tips to conduct a series of tip approach simulations.

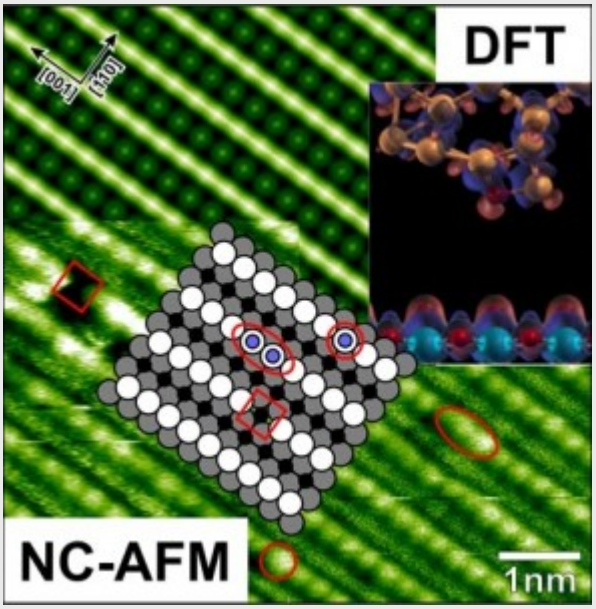
The effect of tip changes on imaging modes was explored by considering tips of different reactivity. Our simulations, in comparison with AFM experimental images, identified a contaminated tip with a Cu-terminated experimental configuration. Charge density and current calculations further helped us investigate the STM imaging modes for tips of different reactivity. Through this work, were able to explain a large variety of experimental STM contrasts obtained. Lastly, simulations of different surface defect models enabled us to understand detailed STM image features and led us to consider the mechanisms of domain formation on the Cu(100)-O surface.

[1] B. J. Albers et al., Nature Nanotech. 4, 307 (2009)
[2] Y. Sugimoto et al., Nature 446, 64 (2007)
[3] P. Jelinek et al, Phys. Rev. Lett. 101, 176101 (2008)
[4] J. M. Blanco, F. Flores and R. Pérez, Prog. Surf. Sci. 81, 403 (2006)

Understanding nc-AFM contrast on TiO2 and water adsorption on CeO2

Wednesday, 14th March 2012. 12:00-13:00

Delia Fernández-Torre



Departamento de Física Teórica de la Materia Condensada, UAM

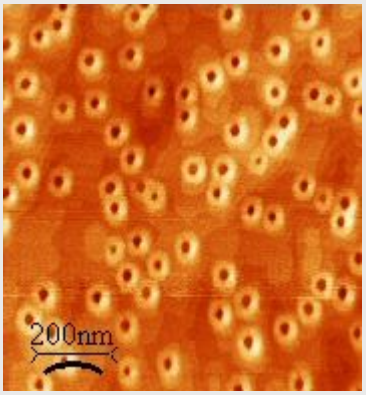
ABSTRACT:
Metal oxides are important for a wide range of technological applications [1]. In order to optimize these proccesses or find new ones it is essential to understand their surface properties and chemistry in detail. Atomically-resolved scanning probe microscopy techniques, like non-contact atomic force microscopy (nc-AFM) [2], combined with theoretical simulations play a crucial role in this respect. In this seminar I will give an overview of our recent and ongoing work on two representative oxide surfaces: TiO2(110) and CeO2(111). I will start by showing how a combination of site-specific force spectroscopy measurements on TiO2(110) and first-principles calculations clarifies the origin of the nc-AFM contrast and let us characterize the tip structures responsible

for the two most common imaging modes [3]. The same model tips can be applied to related systems, like single metal atoms (K, Pt) adsorbed on TiO2(110). I will then consider the problem of water adsorption and pre-dissociation on CeO2(111). When modelling ceria, one has to be specially careful with the approach used for the exchange-correlation functional, as the surface is easily reduced, and the electrons tend to localize on f-states [4]. For water on the clean surface, all our first-principles simulations performed at different levels of theory point to the same solution: water can be adsorbed either molecularly or pre-dissociatively, with adsorption energies in agreement with the experimental data available, and a small barrier (about 0.15 eV) connecting the two structures [5]. Finally, I will show some preliminary results for hydrogen adsorption and dissociation on CeO2(111).
[1] U. Diebold, Surf. Sci. Rep. 48, 53 (2003)
[2] R. García and R. Pérez, Surf. Sci. Rep. 47, 197 (2002)
[3] A. Yurtsever *et al.*, Phys. Rev. B, accepted.
[4] M.V. Ganduglia-Pirovano *et al.*, Surf. Sci. Rep. 62, 219 (2007)
[5] D. Fernández-Torre *et al.*, submitted.

Semiconductor nanostructures grown on GaAs nanoholes for quantum optical information technologies

Wednesday, 7th March 2012. 12:00-13:00

Benito Alén



Instituto de microelectronica de Madrid, CSIC
ABSTRACT:
Single semiconductor quantum dots embedded monolithically in photonic or electronic devices are a fundamental resource for quantum information science and technology.[1] Individual charges and spins can be addressed in these systems through combined electrical and optical manipulation.[2] Quantum information processing tasks can be implemented using the individual spins of a quantum dot molecule as quantum bits.[3] Also, when embedded in a high quality photonic crystal microcavity, spins can be coherently mapped into single photons enabling quantum non-demolition optical read-out or long distance quantum communications.[4]
Despite the considerable progress done so far, standard fabrication methods are based

on self-assembled processes which lead to the random nucleation of the nanostructures over the semiconductor substrate. This is a serious drawback for the deterministic and scalable fabrication of the building blocks mentioned above. In this talk, I will present how semiconductor nanostructures grown directly over pre-patterned substrates could in principle solve this problem. InGaAs quantum dots and quantum dot molecules grown directly on GaAs nanoholes will be presented and their optical and electronic properties will be discussed. [5-8]

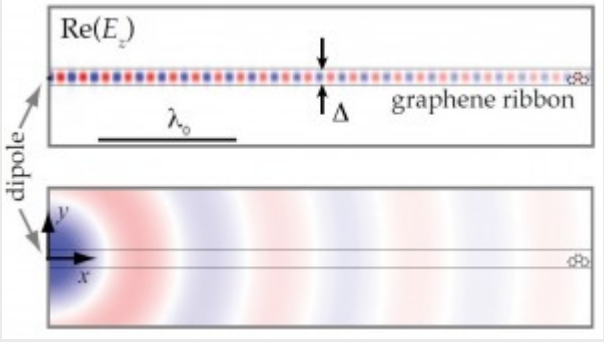
1. Faraon, A. et al. Integrated quantum optical networks based on quantum dots and photonic crystals. New Journal of Physics 13, 055025 (2011).
2. Atature, M. et al. Quantum-Dot Spin-State Preparation with Near-Unity Fidelity. Science 312, 551–553 (2006).
3. Robledo, L. et al. Conditional Dynamics of Interacting Quantum Dots. Science 320, 772 –775 (2008).
4. Rakher, M. T. el al. Externally Mode-Matched Cavity Quantum Electrodynamics with Charge-Tunable Quantum Dots. Phys. Rev. Lett. 102, 097403 (2009).
5. Alonso-González, P. et al. Formation and Optical Characterization of Single InAs Quantum Dots Grown on GaAs Nanoholes. Appl. Phys. Lett. 91, 163104 (2007).
6. Alonso-González, P. et al. Formation of Lateral Low Density In(Ga)As Quantum Dot Pairs in GaAs Nanoholes. Crystal Growth & Design 9, 2525–2528 (2009).
7. Martín-Sánchez, J. et al. Single Photon Emission from Site-Controlled InAs Quantum Dots Grown on GaAs(001) Patterned Substrates. ACS Nano 3, 1513–1517 (2009).
8. Muñoz-Matutano, G. et al. Charge control in laterally coupled double quantum dots. Phys. Rev. B Rapid Comm. 84, 041308 (2011).

Superradiance Mediated by Graphene Surface Plasmons

Wednesday, 29th February 2012. 12:00-13:00

Paloma Arroyo

Departamento de Física Teórica de la Materia Condensada, UAM



ABSTRACT:
As it has been recently shown in two experimental works [1,2], a graphene sheet can support Surface Plasmon Polaritons (SPPs) [3]. Compared to conventional SPPs in metals, the properties of graphene surface plasmons (GSP) can be tuned by means of a gate potential that modifies the conductivity of the electrons in graphene.

In this informal seminar I will talk about the control of the interaction between two emitters mediated by means of the excitation of surface plasmon modes in graphene [4]. First, I will show the emission properties of an emitter close to a graphene sheet and, in particular, the decay through GSP.
Then, I will consider how GSP can be used to tailor the interaction between two emitters. When two emitters are close to a graphene sheet a superradiant state can be achieved where the collective emission is greater than the sum of the individual emissions. Remarkably, due to graphene's properties, the interaction between the emitters can be tuned by means of a gate potential, allowing to change from subradiance to superradiance by modifying the gate.
Moreover, we also study the interaction between two emitters mediated by one-dimensional graphene ribbons supporting waveguide modes [5], which provide a very efficient coupling between two emitters.
[1] Florian Huth, et al, arXiv:1202.4996
[2] Z. Fei1, et al arXiv:1202.4993
[3] A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov, and A. K. Geim, Rev. Mod. Phys. 81, 109 (2009).
[4] Paloma Arroyo Huidobro, A. Y. Nikitin, C. Gonzalez-Ballestero, L. Martín-Moreno, F. J. García-Vidal, arXiv:1201.6492
[5] A. Yu. Nikitin, F. Guinea, F. J. García-Vidal, and L. Martín-Moreno, Phys. Rev. B 84, 161407(R) (2011).

Fano interference and infrared phonon activity in bilayer graphene

Thursday, 23th February 2012. 12:00-13:00

Emmanuele Cappelluti

CNR, Roma & Instituto de Ciencia de Materiales de Madrid, CSIC
ABSTRACT:
The detection and analysis of the spectral properties of optical phonon in single-layer and multilayer graphene provides a powerful tool not only for a careful characterization

of the systems but also for investigating the role of the underlying electron-phonon interaction.
Recent experiments in gated bilayer graphene revealed a clear phonon resonance at 1590 cm-1 with several interesting features, as for instance a giant enhancement of the phonon intensity as a function of teh gate voltage as well as a pronounced Fano lineshape asymmetry.
In this talk I will discuss how these features can be analyzed and predicted on a microscopic quantitative level using a charge-phonon theory applied to the specific case of graphene systems.
We show in particular how the phonon intensity and the Fano asymmetry are strictly related, stemming out from the quantum interference between the electronic and phononic degrees of freedom.
Within this context we are also able to elucidate the relative role of the Eu and Eg phonon modes in regards to the infrared activity and the Fano asymmetry of the observed phonon peaks.
We present thus a complete phase diagram for the strength of the phonon modes and their Fano properties as functions of the chemical potential and of the gated-induced electronic gap, showing that a switching mechanism between the dominance of the Eu or Eg mode can be controlled by the external gate voltage.
Our work permits thus reconciling within a unique theoretical approach the phonon-peak features observed by different experimental groups, and it provides an analytical tool for predicting and controlling on a quantitative level the spectral properties of the phonon resonances in the infrared spectra of graphenes.