The Abdus Salam
International Centre
for Theoretical Physics

17th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods

15 - 17 January 2015

(Miramare, Trieste, Italy)

Co-sponsored by:
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C O N T E N T S

P R O G R A M M E

The Abdus Salam International Centre for Theoretical Physics

International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods | (smr 2703)

Thursday, 15 January 2015

08:00 - 09:00 Registration

All those attending the activity are required to complete registration formalities at the desk in the Leonardo da Vinci Building entrance.

Location: Leonardo da Vinci Building, Lobby

09:00 - 10:00 Quantum Chemistry

Convener: Sandro Scandolo (ICTP)

09:00 **Recent Developments in FCIQMC** *30'*
Speaker: Ali ALAVI (MPI Stuttgart)
Material: Abstract

09:30 **The Density-Matrix Quantum Monte Carlo Method** *30'*
Speaker: Matthew FOULKES (Imperial College)
Material: Abstract

10:00 - 10:30 Coffee break

Location: Leonardo da Vinci Building, Lobby

10:30 - 12:00 Low-dimensional Systems

Convener: Francesco Mauri (Universite Pierre et Marie Curie)

10:30 **Monolayer of 1TMoS2: The Thinnest Ferroelectric?** *30'*
Speaker: Sharmila SHIRODKAR (JNCASR, Bangalore)
Material: Abstract

11:00 **Optical spectra of MoS2: dependence on substrate and electron-phonon coupling** *30'*
Speaker: Ludger WIRTZ (Universite Luxembourg)
Material: Abstract

11:30 **Quantum transport in N-doped graphene and in atomic carbon chains** *30'*
Speaker: Jean-Christophe CHARLIER (Universite Louvain)
Material: Abstract

12:00 - 14:00 Lunch break

14:00 - 15:30 Topological Invariants

Convener: Warren Pickett (UC Davis)

14:00 **Topological physics of transition-metal oxide (111)-bilayers** *30'*
Speaker: Satoshi OKAMOTO (ORNL)
Material: Abstract

14:30 **Searching for topological semi--metals in realistic materials** *30'*
Speaker: Xi DAI (Inst. of Physics, CAS)
Material: Abstract

15:00 **Edge states in graphene nanostructures on metal surfaces** *30'*
Speaker: Riccardo MAZZARELLO (RWTH Aachen)
Material: Abstract

15:30 - 16:00 Coffee break

Location: Leonardo da Vinci Building, Lobby

16:00 - 17:30 Excitation Spectra

Convener: Ralph Gebauer (ICTP)

16:00 **Electronic, optical and vibronic coupling in organic systems from many-body perturbation theory** *30'*
Speaker: Xavier BLASE (Institut Neel, Grenoble)
Material: Abstract

16:30 **Ab initio description of exciton dispersion** *30'*

Speaker: Francesco SOTTILE (Ecole Polytechnique)
Material: Abstract

17:00 **Spectroscopic properties beyond standard GW** *30'*
Speaker: Johannes LISCHNER (Imperial College)
Material: Abstract

18:00 - 20:00 Poster Session

An informal buffet will be served to all participants during the poster session.

Friday, 16 January 2015

09:00 - 10:00 In Honor of David Vanderbilt
Convener: Shobhana Narasimhan (JNCASR)

09:00 **DAVID VANDERBILT@60, And his influence on recent theories of electron-phonon interactions and superconductivity** *1h0'*
Speaker: Marvin COHEN (UC Berkeley)
Material: Abstract

10:00 - 10:30 Coffee break
Location: Leonardo da Vinci Building, Lobby

10:30 - 12:00 First-Principles Simulations
Convener: Steven Louie (University of California at Berkeley)

10:30 **Seeing the covalent bond: Simulating Atomic Force Microscopy Images** *30'*
Speaker: Jim CHELIKOWSKY (U of Texas)
Material: Abstract

11:00 **Quantum-size effects on vibrations and electron-phonon coupling in thin Pb(111) films** *30'*
Speaker: Rolf HEID (KIT Karlsruhe)
Material: Abstract

11:30 **Electric field at the microscopic level: from water dissociation to Miller-like experiments** *30'*
Speaker: Marco SAITTA (Universite Pierre et Marie Curie)
Material: Abstract

12:00 - 14:00 Lunch break

14:00 - 15:30 Molecular Magnets
Convener: Richard Martin (Stanford University)

14:00 **Electronic Structure of Molecular Magnets: Successes within GGA and Challenges for SIC** *30'*
Speaker: Mark PEDERSON (JHU)
Material: Abstract

14:30 **Many-body models for molecular nanomagnets** *30'*
Speaker: Eva PAVARINI (FZ Juelich)
Material: Abstract

15:00 **From molecular magnetism towards molecular spintronics** *30'*
Speaker: Jens KORTUS (TU Freiberg)
Material: Abstract

15:30 - 16:00 Coffee break
Location: Leonardo da Vinci Building, Lobby

16:00 - 17:30 Fundamentals of DFT
Convener: Lucia Reining (Ecole Polytechnique, Palaiseau)

16:00 **Spectroscopic observables from DFT and TDDFT: limitations and hopes** *30'*
Speaker: Stephan KUEMMEL (Universitaet Bayreuth)
Material: Abstract

16:30 **Development and Applications of Potential-Based Density-Functional Theory** *30'*
Speaker: Viktor STAROVEROV (Western University)
Material: Abstract

17:00 **Reduced Density-Matrix Functional Theory: correlation and spectroscopy** *30'*
Speaker: Pina ROMANIELLO (Universite Toulouse)
Material: Abstract

18:00 - 20:00 Poster Session

An informal buffet will be served to all participants during the poster session.

Saturday, 17 January 2015

09:00 - 10:00 **In Honor of Stefano Baroni**

Convener: Nicola Marzari (EPF Lausanne)

09:00 **Water: from deep undercooling to ultrahigh pressure** *1h0'*

Speaker: Roberto CAR (Princeton University)

Material: **Abstract**

10:00 - 11:30 **Interfaces**

Convener: Erik Koch (Forschungszentrum Jülich)

10:00 **Confinement-induced electronic reconstruction in (001) and (111) oriented perovskite superlattices** *30'*

Speaker: Rossitza PENTCHEVA (Universitaet Duisburg-Essen)

Material: **Abstract**

10:30 **First-principles dynamical mean-field perspective on electron correlation and magnetism in oxide heterostructures** *30'*

Speaker: Frank LECHERMANN (Universitaet Hamburg)

Material: **Abstract**

11:00 **Engineering polar discontinuities in honeycomb lattices** *30'*

Speaker: Marco GIBERTINI (EPF Lausanne)

Material: **Abstract**

A B S T R A C T S

O F

I N V I T E D T A L K S

(in alphabetical order)

Recent developments in FCIQMC

Ali Alavi

Max Planck Institute for Solid State Research, Heisenbergstr 1, 70569
Stuttgart, Germany
and
Department of Chemistry, University of Cambridge

We will outline several developments in full Configuration Interaction Quantum Monte Carlo (FCIQMC) methodology which my group has implemented recently. These include a new non-uniform method to generate excitations, which greatly increases the efficiency of the method (while not comprosiming the accuracy), and a method to compute reduced density matrices in an unbiased fashion from the stochastically sampled wavefunction. Applications of the new methodology to the calculation of properties such as nuclear gradients, dipole moments and polarisabilities will be presented. We will also present results on a 3-band model of a strongly correlated cuprate, as well as new benchmark calculations of the ionisation potentials of 3d transition metal atoms.

Electronic, optical and vibronic coupling in organic systems from many-body perturbation theory

Xavier Blase

Institut Néel, CNRS and Grenoble University, Grenoble, France.

The ability of the *GW* and Bethe-Salpeter Green's function many-body perturbation theories to describe the electronic and optical properties of isolated molecules and complexes is being explored by several groups worldwide. While difficulties exist, related e.g. to the starting point dependency, the effect of self-consistency at various levels. or the specific convergence problems for isolated molecules or clusters, we will show that this family of techniques provide reliable results for the description of problematic systems, such as transition-metal containing molecules [1] and the important family of cyanine dyes, [2] or important physical phenomena such as charge transfer excitations [3] and electron-vibration coupling. [4] In the later case, we will summarize in particular our attempts to provide a description of electron-phonon coupling properties within simplified *GW* schemes.

Acknowledgements. Work done in collaboration with C. Faber, P. Boulanger, C. Attaccallite, V. Olévano, and I. Duchemin (Grenoble, France); S. Korbel, M.A.L. Marques, S. Botti (Lyon, France); D. Jacquemin (Nantes, France), D. Beljonne (Mons, Belgium), M. Coté (Montréal, Canada) and E. Runge (Ilmenau, Germany).

References:

[1] S. Korbel *et al.*, J. Chem. Theory Comput. **10**, 3934 (2014).

[2] P. Boulanger *et al.*, J. Chem. Theory Comput. **10**, 1212 (2014); P. Boulanger *et al.*, J. Chem. Theory Comput. **10**, 4548 (2014).

[3] X. Blase, C. Attaccalite, Appl. Phys. Lett. **99**, 171909 (2011); I. Duchemin, T. Deutsch, X. Blase, Phys. Rev. Lett. **109**, 167801 (2012); I. Duchemin and X. Blase, Phys. Rev. B **87**, 245412 (2013); C. Faber *et al.*, J. Chem. Phys. **139**, 194308 (2013).

[4] C. Faber *et al.*, Phys. Rev. B **84**, 155104 (2011); S. Ciuchi *et al.*, Phys. Rev. Lett. **108**, 256401 (2012).

Water: from deep undercooling to ultrahigh pressure

Roberto Car,
Princeton University, Princeton, New Jersey 08544, USA

The structure and dynamics of water change dramatically with mutated thermodynamic conditions, from glassy polymorphs, to metastable and stable liquids, all the way to superionic ice forms at extreme pressure and temperature. The huge range of time scales that characterizes these different states of matter cannot be spanned by a unique simulation approach, but requires models with different levels of coarse graining, ranging from continuous random networks and empirical force fields to ab-initio molecular dynamics approaches.

Quantum transport in N-doped graphene and in atomic carbon chains

Andrés R. Botello-Méndez, Aurélien Lherbier and Jean-Christophe Charlier

University of Louvain, Institute of Condensed Matter and Nanosciences, Belgium

The incorporation of foreign atoms into graphene has been widely investigated in order to modify its electronic and chemical properties. In contrast with conventional materials, the effect of foreign atoms in a 2D material is expected to depend significantly on the position and the local environment of each atom due to the quantum confinement of the electrons. When a nitrogen source is introduced during the CVD growth of graphene, the nitrogen incorporation exhibits a preferential accommodation within one of the two triangular sublattices that compose the honeycomb network [1]. *Ab initio* STM images and computed local density of states reveal specific signatures for each type of nitrogen defects, which are then correlated with experimental STM/STS measurements, thus confirming such a unbalanced sublattice N-doping in graphene (although not hitherto understood). Electronic structure and transport properties of N-doped graphene with a single sublattice preference are then investigated using both first-principles techniques and a real-space Kubo-Greenwood approach [2]. Such a breaking of the sublattice symmetry leads to the appearance of a true band gap in graphene electronic spectrum even for a random distribution of the N dopants. In addition, a natural spatial separation of both types of charge carriers at the band edge is observed, leading to a highly asymmetric electronic transport. For such N-doped graphene systems, the carrier at the conduction band edge present outstanding transport properties including long mean free paths, high mobilities and conductivities. Such a transport behavior can be explained by a non-diffusive regime (quasi-ballistic transport behavior at the conduction band edge), and originates from a low scattering rate [2]. The presence of a true band gap along with the persistence of carriers traveling in an unperturbed sublattice suggest the use of such N-doped graphene in G-FET applications, where a high I_{ON}/I_{OFF} ratio is expected. The present *ab initio* simulations should encourage more investigation and specific transport measurements on N-doped graphene samples where such an unbalanced sublattice doping is observed.

Carbyne, the sp^1-hybridized phase of carbon, is still a missing link in the family of carbon allotropes. Despite many efforts in synthetic chemistry, bulk phases of carbyne remain elusive, and this type of carbon material is believed to be unstable. However, in recent years the elementary constituents of carbyne, i.e., linear chains of carbon atoms, have been observed in the electron microscope. Hence, isolated atomic chains exist and are highly interesting one-dimensional conductors that have stimulated considerable theoretical work. Because of the challenge involved in the controlled synthesis and characterization of carbon chains, experimental information is still very limited. Recently, detailed electrical measurements and first-principles electronic transport calculations have been performed on monoatomic carbon chains [3-4]. When the 1D system is under strain, the current-voltage curves exhibit a semiconducting behavior, which corresponds to the polyyne structure of the atomic chain with alternating single and triple bonds. Conversely, when the chain is unstrained, the ohmic behavior is observed in agreement with the metallic cumulene structure with double bonds. This confirms a recent theoretical prediction, namely that a metal-insulator transition can be induced by adjusting the strain. The key role of the contacting leads is also scrutinized by *ab initio* quantum conductance calculations, explaining the rectifying behavior measured in monoatomic carbon chains in a non-symmetric contact configuration.

[1] R. Lv, Q. Li, A.R. Botello-Mendez, *et al.*, Scientific Reports **2**, 586 (2012)

[2] A. Lherbier, A.R. Botello-Mendez, and J.-C. Charlier, Nano Lett. **13**, 1446 (2013)

[3] O. Cretu, A.R. Botello-Mendez, I. Janowska, C. Pham-Huu, J.-C. Charlier, and F. Banhart, Nano Lett. **13**, 3487 (2013)

[4] A. La Torre, A.R. Botello-Mendez, W. Baaziz, J.-C. Charlier, and F. Banhart, submitted (2014)

Seeing the covalent bond: Simulating Atomic Force Microscopy Images

James R. Chelikowsky

Center for Computational Materials, Institute of Computational Engineering and Sciences, Departments of Physics and Chemical Engineering, University of Texas at Austin, Austin, Texas 78712 USA

Advances in atomic force microscopy (AFM) have made it possible to achieve unprecedented images of covalent bonds, in some cases even to resolve the bond order in polycyclic aromatics. However, fundamental questions remain about interpreting the images and modeling the AFM tip. For example, the bright spots in non-contact AFM images can have a close correspondence to the atomic structure of a given specimen, but there can be contrast changes with tip height that cannot be interpreted directly by atomic positions. While the nature of the tip can be crucial in understanding the details of the image, the atomic structure of the tip is often unknown. This situation is compounded by the difficulty in simulating AFM images. In order to perform computational studies of AFM, one must determine the interatomic forces as a function of the tip height on a fine grid above the specimen.

We propose new high performance algorithms to solve for the quantum forces between the tip and the specimen. This approach coupled with a simple theory that avoids an explicit model of the AFM tip, allows us to accurately replicate AFM images and resolve outstanding issues in their interpretation.

References: T.-L. Chan, C.Z. Wang, K.M. Ho, J.R. Chelikowsky:"Efficient first-principles simulation of noncontact atomic force microscopy for structural analysis," Phys. Rev. Lett. 102, 176101 (2009) and M. Kim and J.R. Chelikowsky: "Simulated non-contact atomic force microscopy for GaAs surfaces based on real-space pseudopotentials," Appl. Surf. Sci. 303,163 (2014).

"DAVID VANDERBILT@60, AND HIS INFLUENCE ON RECENT THEORIES OF ELECTRON-PHONON INTERACTIONS AND SUPERCONDUCTIVITY"

Marvin L. Cohen

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University of California at Berkeley
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At this 2015 Electronic Structure/Computational Materials Physics Workshop here in Trieste, it is a great pleasure for me to contribute to the sessions in honor of the 60th birthdays of David Vanderbilt and Stefano Baroni. Roberto Car will discuss the career of Stefano Baroni, and I will describe some of David Vanderbilt's contributions to condensed matter physics. In particular, I will focus on David's creative use of Wannier functions which has had a big impact. I'll discuss how this new emphasis on Wannier functions led to important advances related to studies of electron-phonon interactions and superconductivity.

Searching for topological semi-metals in realistic materials

Xi Dai

Division of Theory, The Institute of Physics, Chinese Academy of Sciences, #8 South Third Street, 100190 Beijing, China

Topological semi-metal (TSM) is a new type of quantum phases in condensed matter, which includes Dirac semi-metal (DSM) and Weyl semi-metal (WSM) phases. The appearance of DSM phase requires additional crystal symmetry to generate Dirac points along some special directions. And the WSM phase requires breaking of either time reversal or inversion symmetry to remove the spin degeneracy. In the present talk, I will summarize the TSM materials found recently in our group by first principle methods. Besides the exotic physical properties of these TSMs, I will also introduce from the symmetry point of view where and how to find these materials.

The Density-Matrix Quantum Monte Carlo Method

W.M.C. Foulkes, N.S. Blunt, T.W. Rogers, F. Malone, J.S. Spencer
Department of Physics, Imperial College London

J.J. Shepherd
Rice University

The density-matrix quantum Monte Carlo (DMQMC) method [1] is a finite-temperature generalization of the full-configuration-interaction quantum Monte Carlo (FCIQMC) method recently introduced by Booth, Thom and Alavi [2]. Like FCIQMC, DMQMC overcomes the fermion sign problem in small enough systems. Unlike FCIQMC, which is primarily a ground-state method, DMQMC samples the density operator of a many-particle system at finite temperature. The availability of the density matrix allows arbitrary reduced density matrix elements and expectation values of complicated non-local observables to be evaluated. This talk explains the theory behind DMQMC, describes the algorithm, and introduces an importance-sampling procedure to improve the stochastic efficiency. To demonstrate the potential of DMQMC, the energy and staggered magnetization of the isotropic antiferromagnetic Heisenberg model on small lattices, the concurrence of one-dimensional spin rings, and the Renyi S_2 entanglement entropy of various sublattices of the 6×6 Heisenberg model are calculated. We also present preliminary results for warm dense electron gas systems.

[1] N.S. Blunt, T.W. Rogers, J.S. Spencer, and W.M.C. Foulkes, Phys. Rev. B **89**, 245124 (2014)

[2] G.H. Booth, A.J.W. Thom, and A. Alavi, J. Chem. Phys. **131**, 054106 (2009)

Engineering polar discontinuities in honeycomb lattices

Marco Gibertini

Theory and Simulation of Materials (THEOS) and National Center for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, Switzerland

Unprecedented and fascinating phenomena have been recently observed at oxide interfaces between centrosymmetric cubic materials, where polar discontinuities can give rise to polarization charges and electric fields that drive a metal-insulator transition and the appearance of a two-dimensional electron gas. Lower dimensional analogues are possible, and honeycomb lattices offer a fertile playground thanks to their versatility and the extensive on-going experimental efforts in graphene and related materials. Here we suggest different realistic pathways to engineer polar discontinuities in honeycomb lattices, and support these suggestions with extensive first-principles calculations. Several approaches are discussed, based on (i) nanoribbons, where a polar discontinuity against the vacuum emerges, and (ii) functionalizations, where covalent ligands are used to engineer polar discontinuities by selective or total functionalization of the parent systems. All the cases considered have the potential to deliver innovative applications in ultra-thin and flexible solar-energy devices and in micro- and nano-electronics.

Quantum-size effects on vibrations and electron-phonon coupling in thin Pb(111) films

Rolf Heid

Institute for Solid State Physics, Karlsruhe Institute of Technology, Germany

Thin metal films are well known realizations of the geometrical confinement of electronic motion which manifests itself in the presence of quantum-well states and profoundly alters the electronic structure. Its influence on the electron-phonon coupling is, however, much less understood. In this context, Pb(111) films on semiconducting substrates have been studied extensively in recent years, because superconductivity was found to persist in ultrathin films, albeit with reduced transition temperature [1], and was observed even for a single monolayer [2]. This raised questions to what extend quantum-size effects modify the electron-phonon coupling directly, and what is the role of the substrate.

In this talk, I will present a comprehensive first principles investigation of electronic, vibrational, and electron-phonon coupling (EPC) properties of thin Pb(111) films in the framework of density functional perturbation theory. Similar to the findings for lead bulk [3], it was imperative to include spin-orbit interaction for a proper quantitative description of vibrational spectra and coupling strengths. Results for Fermi surface averaged couplings, relevant for superconductivity [4], as well as for EPC-induced self-energies of quantum well states for various film thicknesses are discussed in comparison with recent experiments. I will also address the influence of the substrate on these properties.

[1] Y. Guo *et al.*, Science **306**, 1915 (2004)
[2] T. Zhang *et al.*, Nat. Phys. **6**, 104 (2010)
[3] R. Heid *et al.*, Phys. Rev. B **81**, 174527 (2010)
[4] I.Yu. Sklyadneva *et al.*, Phys. Rev. B **87**, 085440 (2013)

From molecular magnetism towards molecular spintronics

Jens Kortus

TU Bergakademie Freiberg, Leipziger Str. 23, D-09599 Freiberg, Germany

In the first part of my talk I will discuss how calculations based on density functional theory (DFT) can guide qualitatively (or sometimes even quantitatively) in the design of molecules with improved magnetic anisotropy barrier [**?**].
In the second part I will focus on metal-phthalocyanines (MPc), which are promising molecular materials for spintronics. Electronic structure calculations can provide information required for interpretations of experimental data. In particular a recently investigated layered system of MnPc and F_{16}CoPc shows charge transfer at the interface between the MPc's. DFT calculations reveal that a hybrid state is formed between the two types of phthalocyanines, which causes this charge transfer. For the hybrid state the Mn $3d_{xz}$ interacts with the Co $3d_{z^2}$ orbital leading to a two-level system [**?**, **?**, **?**].
These results are of importance for the application of such interfaces in organic electronic devices since charge transfer considerably affects the energy level alignment and the transport behaviour of the respective hetero-junction. Since the transfer of charge is also connected to a transfer of spin and the hybrid system has a net spin of $S = 2$, such compounds could also be termed *spin-transfer materials* with future applications in the area of spintronics.

References

[1] J. Cirera, E. Ruiz, S. Alvarez, F. Neese, J. Kortus, Chem.-Eur. J. **15**, 4078 (2009); E. Ruiz, J. Cirera, J. Cano, S. Alvarez, C. Loose, J. Kortus, Chem. Commun. **1**, 52 (2008)

[2] S. Lindner, M. Knupfer, R. Friedrich, T. Hahn and J. Kortus, Phys. Rev. Lett. **109**, 027601 (2012)

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[4] R. Friedrich, B. Kersting, J. Kortus, Phys.Rev. B **88**, 155327 (2013)

Spectroscopic observables from DFT and TDDFT: limitations and hopes

Stephan Kümmel

Theoretical Physics IV, University of Bayreuth, Bayreuth, Germany

Present day density functionals serve many purposes, but most of them also suffer from systematic limitations. The insufficient accuracy in describing localization effects, the tremendous overestimation of long-range charge transfers, and the limited interpretability of the Kohn-Sham eigenvalues are prominent examples. This talk will show that many of these problems are inherently linked to one-electron self-interaction and can be significantly reduced with a self-interaction correction based on the Optimized Effective Potential [1]. It will further be discussed that range-separated hybrid functionals can achieve similar effects in a different way. Pros and cons of both type of approaches will be pointed out [2,3]. Final remarks will address the hopes that one may pin on new types of semi-local functionals which capture important features of exact exchange in their semi-local potential [4].

[1]
D. Hofmann, T. Körzdörfer, S. Kümmel,
"Kohn-Sham Self-Interaction Correction in Real Time",
Physical Review Letters 108, 146401 (2012).

[2]
A. Karolewski, L. Kronik, S. Kümmel,
"Using optimally tuned range separated hybrid functionals in ground-state calculations: Consequences and caveats",
J. Chem. Phys. 138, 204115 (2013)

[3]
Thiago B. de Queiroz, S. Kümmel,
"Charge-transfer excitations in low-gap systems under the influence of solvation and conformational disorder: Exploring rang-separation tuning",
Journal of Chemical Physics 141, 084303 (2014)

[4]
R. Armiento, S. Kümmel,
"Orbital Localization, Charge Transfer, and Band Gaps in Semilocal Density-Functional Theory",
Physical Review Letters 111, 036402 (2013)

First-principles dynamical mean-field perspective on electron correlation and magnetism in oxide heterostructures

Frank Lechermann

I. Insitute for Theoretical Physics, University of Hamburg, Germany

The investigation of oxide heterostructures provides the possibility for exploring novel composite materials beyond nature's original conception (see [1] for a recent review). Emerging electronic phases within the interface region between e.g. bulk compounds of band- and/or Mott-insulating character pose a formidable problem beyond the scope of either conventional density functional theory (DFT) or minimal model-Hamiltonian approaches. By means of the charge self-consistent combination of DFT with dynamical mean-field theory (DMFT) an advanced realistic many-body methodology is available that may tackle this challenge. In this talk the theoretical framework will be presented and the application to intricate heterostructure problems discussed.

I thereby mainly focus on two concrete problems. First, the δ-doping of distorted-perovskite Mott-insulating titanates with a single SrO layer along the [001] direction gives rise to a rich correlated electronic structure [2]. From a realistic superlattice study, layer- and temperature-dependent multi-orbital metal-insulator transitions are revealed. Furthermore, breaking the spin symmetry in δ-doped $GdTiO_3$ results in blocks of ferromagnetic itinerant and ferromagnetic Mott-insulating layers which are coupled antiferromagnetically. Second, DFT+DMFT insight [3] into the metallic state and the key mechanism for itinerant ferromagnetism at the band-band insulating $LaAlO_3/SrTiO_3$ interface will be provided.

[1] J. Chakhalian, J. W. Freeland, A. J. Millis, C. Panagopoulos and J. M. Rondinelli, RMP 86, 1189 (2014) [2] F. Lechermann and M. Obermeyer, arXiv:1411.1637 (2014) [3] F. Lechermann, L. Boehnke, D. Grieger and C. Piefke, PRB 90, 085125 (2014)

Spectroscopic properties beyond standard GW

Johannes Lischner
Department of Physics and Department of Materials, Imperial College London.

Spectral functions are measured in photoemission and tunneling experiments. The GW method is the state-of-the-art approach to calculate spectral functions that include many-electron interaction effects beyond density-functional theory. While GW theory has been very successful for the description of quasiparticle excitations in a wide range of physical systems including semiconductors and insulators, other systems and properties require going beyond the standard formalism.
For open-shell systems, such as magnetic molecules or magnetic defects in solids, I have developed a Green's function approach based on the GW approximation. In these systems, the poles of the self energy give rise to the characteristic multiplet structure observed in photoemission experiments. For the calculation of plasmon satellite features in spectral functions, GW plus cumulant theory cures the failure of GW theory which is known to significantly overestimate the separation of quasiparticle and satellite peaks. Finally, I present a first-principles approach to include the coupling of quasiparticles to spin fluctuations, which play an important role in metals, magnets and unconventional superconductors.

Edge states in graphene nanostructures on metal surfaces

Riccardo Mazzarello

Institute for Theoretical Solid State Physics and JARA, RWTH Aachen University, Germany

Graphene is a fascinating two-dimensional system with unique electronic and transport properties. Nevertheless, the absence of an energy gap in its band structure limits its applicability in semiconductor technology. Fabrication of graphene nanostructures, such as nanoribbons and quantum dots, provides a route to induce the required band gap. Interestingly, zigzag-terminated nanostructures possess electronic states localized at the edge, which lead to non-trivial magnetic properties. In fact, in the case of graphene nanoribbons, mean field calculations predict a ferromagnetic spin polarization along the two edges and an antiferromagnetic coupling across the nanoribbon. These properties have been investigated intensively recently, due to potential applications in the field of spintronics. However, in principle, there exist various effects which can undermine the stability of edge magnetism, including quantum and thermal fluctuations, edge reconstruction and passivation, and, for supported nanostructures, the interaction with the substrate.

In this work, we have focused on substrate effects. For this purpose, we have carried out a density functional theory study of the electronic and magnetic properties of graphene nanoribbons on the (111) surface of several metallic substrates, namely Ir, Au, Ag and Cu. The selected substrates are commonly used to grow graphene nanostructures by chemical vapor deposition methods or bottom-up approaches. We have considered both H-free and H-passivated nanostructures. In the case of the Ir(111) surface, we do not find states localized at the nanoribbon edges. We explain this result by the interplay between a strong and intricate hybridization of the graphene π orbitals with Ir d states and a lattice-mismatch driven geometrical relaxation at the edges. Our simulations are in agreement with scanning tunneling spectroscopy experiments performed on graphene islands on Ir(111). In the case of Au, Ag and Au substrates, the nanoribbons possess edge states. In spite of this, they do not exhibit a significant magnetization at the edge, with the exception of H-terminated nanoribbons on Au(111), whose zero-temperature, mean-field magnetic properties are comparable to those of free-standing nanoribbons. These findings are explained in terms of the different chemical interaction and charge transfer between the nanoribbons and the three substrates.

Topological physics of transition-metal oxide (111)-bilayers

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Transition metal oxides (TMOs) have long been one of the main subjects of material science because of their novel functionalities such as high-T_c superconductivity in cuprates and the colossal magnetoresistance effect in manganites. A new era for the study of novel oxides was opened by the recent developments in thin film growth techniques with the atomic precision. A variety of heterostructures involving TMOs have been fabricated and characterized, leading to, for example, the discovery of two-dimensional electron gases, magnetism, and superconductivity at interfaces between two dissimilar insulators. Further novel phenomena could emerge in such TMO heterostructures. In this talk, I will present our theoretical work designing band topology using oxide heterostructures. Specifically, I consider bilayers of TMOs grown along the [111] crystallographic axis. A variety of novel phenomena are predicted, including quantum spin Halll effects [1] and anomalous Hall effects [2]. The effects of many-body interactions are discussed by means of a slave-boson mean-field method [3] and the dynamical-mean-field theory [4]. This work is supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

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Many-body models for molecular nanomagnets

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I will present a novel [1] flexible and effective scheme to build *ab-initio* many-body models –and the corresponding low-energy magnetic Hamiltonians– for molecular nanomagnets. It is based on using localized Foster-Boys orbitals as a one-electron basis. I will illustrate applications of this scheme to some paradigmatic systems: the antiferromagnetic rings Cr_8 and Cr_7 Ni, the single-molecule magnet Fe_4, and two Cr_7Ni-Ni-Cr_7Ni assemblies [1,2].

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Electronic Structure of Molecular Magnets: Successes within GGA and Challenges for SIC

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The experimental observation of resonant tunneling of magnetization in molecular magnets has led to significant theoretical interest in the first-principles electronic-structure based understanding of the magnetic- and spin-dependent- processes in these systems. For cases where the electronic structure is described qualitatively correctly, the PBE-GGA has been rather successful in accurately predicting many-of the molecular magnets composed of 3d-transition metal ions. Predictive successes include quantitative determination of magnetic reorientation barriers and the qualitatively correct description of the spin-excitation spectrum. This talk will highlight some of these successes[1,2] but focus on identifying challenging molecular-magnetic systems where the use of self-interaction corrected versions of density-functional theory is expected to lead to better predictive capabilities. For example for the Cu_3 and V_{15} molecular magnets, both of which simplify to a frustrated equilateral triangle of three spin $\frac{1}{2}$ transition-metal cations, the PBE-GGA provides the correct low-energy spin states but overestimates the splittings between the low-lying Kramer doublets and the upper quartet due to the slightly delocalized d-electrons on the transition-metal sites[1]. Rationale for why electronic-structure calculations with self-interaction-corrected functionals, could improve spin-excitations will be discussed. In regard to understanding spin-dependent electron transfer across molecular magnets, it is necessary to accurately calculate the charge states of a molecular magnet that is tethered to a distant electrode by a polymer. Through applications of DFT involving to Mn_{12} and Fe_4 molecular magnets as possible circuit elements and gold- and spin-polarized graphene flakes as possible substrates, the relation of the level alignment problem to the self-interaction correction will be highlighted. A new unitarily-invariant method for efficiently and exactly accounting for the self-interaction corrections for all electrons, with applications to simple transition-metal systems will be briefly introduced and discussed[3]. [1]MR Pederson and SN Khanna, Phys. Rev. B **60**, 9566 (1999), [2]J. F Nossa, MF Islam, CM Canali and MR Pederson, PRB **85** 085427 (2012). [3]M. R. Pederson, A. Ruzsinszky, and J. P. Perdew, J. Chem. Phys. **140**, 121103 (2014).

Confinement-induced electronic reconstruction in (001) and (111) oriented perovskite superlattices

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Oxide interfaces exhibit a broad spectrum of functional properties that are not available in the respective bulk compounds, such as two-dimensional conductivity, superconductivity and magnetism. In this talk I will compare the mechanisms of electronic and orbital reconstruction in oxide quantum wells with (001) and (111) crystallographic orientation. The latter promise to host even more exotic electronic states compared to the much studied (001)-oriented systems due to their distinct topology [1]. Material-specific density functional theory calculations with an on-site Coulomb repulsion term are used to explore the role of confinement, symmetry breaking, polarity mismatch and strain in the emergence of novel electronic phases. The results illuminate a rich set of competing ground states in polar $(LaAlO_3)_M/(SrTiO_3)_N(111)$ [2] and non-polar $(LaNiO_3)_M/(LaAlO_3)_N(111)$ [3,4] superlattices, ranging from spin-polarized, Dirac-point Fermi surfaces protected by lattice symmetry to charge-ordered Mott or Peierls insulating phases. Analogous to the (001) counterparts [5,6], orbital reconstructions and metal-to-insulator transitions depend critically on the thickness of the quantum well and in-plane strain, thus opening avenues for engineering properties at the nanoscale.
Research in collaboration with D. Doennig, A. Blanca-Romero and W.E. Pickett; supported by the DFG, SFB/TR80.

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Reduced Density-Matrix Functional Theory: correlation and spectroscopy

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In this work we explore the performance of approximations to electron correlation in reduced density-matrix functional theory (RDMFT) [1] and of approximations to the observables calculated within this theory. Our analysis focuses on the calculation of total energies, occupation numbers, removal/addition energies, and spectral functions. We use the exactly solvable Hubbard molecule at 1/4 and 1/2 filling as test systems. This allows us to analyze the underlying physics and to elucidate the origin of the observed trends. For comparison we also report the results of the *GW* approximation, where the self-energy functional is approximated, but no further hypothesis are made concerning the approximations of the observables. In particular we focus on the atomic limit, where the two sites of the molecule are pulled apart and electrons localize on either site with equal probability, unless a small perturbation is present: this is the regime of strong electron correlation. In this limit, using the Hubbard molecule at 1/2 filling with or without a spin-symmetry-broken ground state, allows us to explore how degeneracies and spin-symmetry breaking are treated in RDMFT. We find that, within the used approximations, neither in RDMFT nor in *GW* the signature of strong correlation are present in the spin-singlet ground state, whereas both give the exact result for the spin-symmetry broken case. Moreover we show how the spectroscopic properties change from one spin structure to the other. Our findings can be generalized to other situations, which allows us to make connections to real materials and experiment. [2]

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Electric field at the microscopic level: from water dissociation to Miller-like experiments

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In the last decade, thanks to Berry-phase theory and its implementation in DFT schemes, it is possible to study the effect of finite homogenous electric fields in ab initio molecular dynamics simulations [1]. Here we present a study of bulk liquid water under intense electric fields [2]. We observe that the hydrogen-bond length and the molecular orientation are significantly modified at low-to-moderate field intensities. Fields beyond a threshold of about 0.35 V/Å are able to dissociate molecules and sustain an ionic current via a series of correlated proton jumps, in good agreement with experimental values [3]. Upon applying even more intense fields ($\sim$ 1.0 V/Å), a 15%-20% fraction of molecules are instantaneously dissociated and the resulting ionic flow yields a conductance of about 7.8 Ω^{-1} cm^{-1}. We then undertake the first ab initio computer simulations of the celebrated Miller experiment, that we perform in the condensed phase [4] Our study shows that glycine spontaneously forms from mixtures of simple molecules once an electric field is switched on. Moreover, combining the electric field approach with a metadynamics-based analysis of chemical reactions[5], we identify formic acid and formamide as key intermediate products of the early steps of the Miller reactions, and the crucible of formation of complex biological molecules.

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Monolayer of 1TMoS$_2$: The Thinnest Ferroelectric?

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Ferroelectric crystals exhibit an electric dipole moment (spontaneous polarization) even in the absence of an external electric field. When heated, ferroelectric materials transform at the ferroelectric transition temperature to the centrosymmetric and non-polar paraelectric phase. The macroscopic electric polarization in ferroelectrics can be switched by the application of external electric fields. Hence, their films are used in various devices such as sensors, actuators and memories. As ferroelectric ordering of dipoles oriented perpendicular to the surface of an ultrathin film is suppressed by their depolarization field, ferroelectricity has been shown to disappear below film thicknesses of 24 Å in $BaTiO_3$, 8 Å in $PbTiO_3$ and 10 Å in polymer films. However, truly 2-dimensional materials such as graphene, hexagonal boron nitride and MoS_2 have not been explored for its existence. Here, we predict the emergence of unexpected, yet robust ferroelectricity (with polarization perpendicular to the plane) in the 1T polytype of MoS_2 as it undergoes a transition from metallic to insulating state by using a combination of first-principles and Landau theoretical analysis. We show that it originates from the geometry of electronic Fermi surface through a strong coupling of d-orbitals of Mo with valley phonons that induce an effective electric field. Our prediction of a 2-dimensional ferroelectric semiconductor opens up a new class of nanoscale dipotronic devices based on MoS_2, and we propose XNOR, NAND and OR logic gates within a single transistor structure [1].

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Ab initio description of exciton dispersion

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We present ab initio calculation of plasmon and exciton dispersion of wide-gap insulators, like LiF or hBN, as well as molecular solids. With the help of the Bethe-Salpeter Equation (recently extended [1,2] to describe full coupling momentum excitonic effects) we calculate the momentum dispersion of the first low-lying excitons, both visible and dark. Their particular behaviour is analysed (with respect to momentum intensity and direction, coupling effect, real space distribution and interference effects) and the results are compared with recent inelastic X-ray scattering [3] and with electron energy loss spectroscopy [4,5].

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Development and Applications of Potential-Based Density-Functional Theory

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I will survey recent advances in the theory of Kohn–Sham effective potentials and show how, by thinking in terms of these quantities, one can obtain new physical insights and better density-functional approximations for computing molecular properties. Topics include: development of energy functionals from Kohn–Sham potentials, accurate prediction of excitation energies, and a new tool for studying chemical reactivity called the average local electron energy.

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Optical spectra of MoS_2: dependence on substrate and electron-phonon coupling

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Layered transition-metal dichalcogenides, in particular the semiconducting MoS_2, are attracting currently a lot of attention due to their possible use in thin-film electronics. Also from the fundamental point of view, these materials are very interesting due to their complex band-structure, strong effects of spin-orbit splitting and the possibility of valley polarization by circularly polarized light. We summarize the debate on the quasi-particle band-structure of single and few-layer MoS_2 (self-consistent versus non-self consistent GW). We discuss the influence of slight changes in the geometry of the single-layer as well as of the underlying substrate. Optical absorption spectra are calculated on the level of the Bethe-Salpeter equation including the effect of spin-orbit coupling. Taking into account the effect of electron-phonon coupling, we calculate the temperature dependence of the band gap and the absorption spectra. We discuss the origin of the experimentally observed doubling of the high-energy exciton at 2.6 eV on a gold substrate as the potential effect of a "mirror exciton" (exciton formed from image states).

Following collaborations are gratefully acknowledged: For the theory: Alejandro Molina-Sánchez (Luxembourg), Maurizia Palummo, Davide Sangalli, Andrea Marini (Rome), and Kerstin Hummer (Vienna). For the experimental work on the mirror excitons: Jan Mertens, Jeremy J. Baumberg (Cambridge), Yumeng Shi, Hui Ying Yang (Singapore).

TITLES OF ABSTRACTS OF POSTERS

POSTER SESSION I

THURSDAY, 15 JANUARY 2015

The full abstract can be found on the Workshop's website:

http://indico.ictp.it/event/a14243

POSTER SESSION I

THURSDAY, 15 JANUARY 2015

In alphabetical order of presenting author (underlined)

Study of Electronic Properties of BC2N Nanotubes

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Ab initio study of the Ni-Graphene interface: the role of screened van der Waals interactions

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Electrostatics of solvated systems in periodic boundary conditions

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Structural and electronic properties of Polyacetylene chains through Variational Monte Carlo

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Solvation effects on the color optical properties of anthocyanin natural dyes

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Solution of the many-body problem in one point

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First-principles study of structure, vibrational and elastic properties of stoichiometric and calcium-deficient hydroxyapatite

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Defect states of Mn, Fe, and V:Ga in GaN: comparing GGA+U with experiment

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Ab-initio study of dynamical stability and anharmonic effects in high pressure metallic atomic hydrogen

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Sovated low bandgap oligomers: Challenges and advances in Density Functional Theory

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Light-induced field enhancement in polyacenes

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Transparent Conductive Oxides as Near-IR Plasmonic Materials for Energy Conversion

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Atomistic simulations of thermal transport and thermal boundary resistance in phase change materials for non-volatile memories

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Surface-assisted formation of grapheme nanoribbons on Au surfaces

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Electron energy loss anisotropies in MAX phases: Ti2AlC

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Phonon Hydrodynamics in Two-Dimensional Materials

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Density Functional Theory study of highly excited ultra-cold atoms in a periodic lattice

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Designing FePt-Fe3Pt hard-soft magnetic composite materials from ab initio calculations

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Searching for high magnetization density in bulk Fe: the new metastable Fe6 phase

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Imaging electron correlation in molecules by scanning tunneling microscopy: an ab-initio prediction

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DFT study of the reactivity of CO2 in molten alkali carbonates

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Clean Ir(111) and Pt(111) electronic surface states: a first-principle fully relativistic investigation

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First-principles study of Radical Organic Electrodes

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On the interpretability of molecular orbitals from organic semiconductors

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Transport Properties of Iron-Porphyrin / Graphene Junction

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Thermoelastic properties of α-iron: model potentials and first-principles calculations

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Efficient ab initio calculation of anharmonic properties in solids: the stochastic self-consistent harmonic approximation

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Thermodynamic integration to monitor parameter convergence in molecular dynamics: application to liquid water

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Thermoelectric properties of n-doped Silicon from first-principles

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A generalized Poisson solver for complex electrostatic environments

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Anchoring and Bending of Pentacene on Aluminum (001)

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Enhanced Atom Mobility on the Surface of a Metastable Film

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Multiphoton k-resolved photoemission from gold surface states with 800-nm femtosecond laser pulses

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Resonant Lifetime of Core-Excited Organic Adsorbates from First Principles

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A general method for functional optimization

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Subsystem Density Functional Theory for Periodic Systems
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Effects of anion doping on oxide-metal interface: a DFT study of MgO/Mo
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Unravelling the origin of the E'α and Ge(2) centers
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Local Reduced Density Matrix Functional Theory
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Magnetic Anisotropy Energy in Narrow Silicene Nanoribbons
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Speeding up linear-response DFT calculations with optimally reduced plane-wave basis sets
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Ferromagnetic iron as a topological metal

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High performance electronic structure engineering with hybrid DFT and GW

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Nonorthogonal generalized hybrid Wannier functions for linear scaling DFT simulations of surfaces and interfaces

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Electronic properties and van Hove singularities of observed moiré patterns of dislocated graphene on HOPG

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Electronic and Optic Properties of Corrugated Quantum Wells

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Valence Band Structure of Square Quantum Well Under Stress

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Electronic structure of substitutionally disordered systems: orbitalbased CPA within a pseudopotential approach

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Ab initio study of the ferroelectric resistive switching in the LSMO/PZT/Co multiferroic tunnel junction

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A systematically improvable second-pronciples method including electron and lattice degrees of freedom

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Thermoelectricity: Coupling transport equations and _ab initio_ calculation

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Interplay between defects and stacking at the SiC/SiO2 interface

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A General Purpose Massively Parallel _Ab Initio_ Molecular Dynamics Implementation With A Linear Scaling Exact Exchange Algorithm

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First-Principles Study Of Oxide Superlattices

Aysegul Begum Kocak, Marie-Bernadette Lepetit1, Philippe Ghosez2 & Julien Varignon2

Conversion of Toxic H2S to Green Fuel H2 with 2D-ZnO1-xNy

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Metal-Insulator Transition and Lattice Instability of Paramagnetic V2O3

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POSTER SESSION II

FRIDAY, 16 JANUARY 2015

The full abstract can be found on the Workshop's website:

http://indico.ictp.it/event/a14243

POSTER SESSION II

FRIDAY, 16 JANUARY 2015

In alphabetical order of presenting author (underlined)

Atomistic simulations of multicaloric effects in ferroelectrics
S. Lisenkov and I. Ponomareva
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Structural defects in P3HT-polymer chains probed in the ballistic transport regime
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Substrate doping: A strategy for enhancing reactivity of gold nanocatalyst by tuning the sp-bands
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πAg nanoclusters: An ab-initio vibrational dynamics Study
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Thermal properties of bismuth calculated from first principles
Maxime Markov1, Jelena Sjakste1 , Giorgia Fugallo1, Lorenzo Paulatto2, Francesco Mauri2, Michele Lazzeri2, Nathalie Vast1
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The Mixed (L-Threoninato)(L-Aasparaginato)Copper(II) System - Conformational Analysis of an Isolated Complex

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Ultra-fast transient absorption of monolayer MoS2 from first principles

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Projector Augmented-wave formulation of response to strain and electric field perturbation within the density-functional perturbation theory

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Electronic and magnetic structures of semimagnetic semiconductors investigated by first principle, mean field and series expansions calculations

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Surface Adsorbates and Defects on the Subsurface Cation Vacancy Stabilized Surface of Magnetite (001)

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A multiscale computational method for fluid dynamics simulation: application of nanoscience to enhanced oil recovery process

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Stable and Efficient Linear Scaling First-Principles Molecular Dynamics for 10,000+ atoms

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Ab Initio Simulation of Enhanced Phosphorus-based Nano-composite Materials

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An investigation of quantum transport properties in silicon nanotube

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Efficient optimization of local orbitals and eigenstate calculations in linear-scaling DFT code CONQUEST

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Native defects and impurities in single-layer MoS2 and shallow level formation with dielectric environments

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Quantum Confinement in Silicon Quantum-Slabs

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First-Principles Calculation for Thermal Oxidation Process of SiC

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First Principle Simulation of Optical Spectra in Gold-based Alloys

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Enhancement of superconductivity with low doping in two-dimensional multivalley semiconductors

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Jastrow correlations for solids

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Efficient conformational sampling of complex adsorbates with Basin Hopping in curvilinear coordinates

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Surface phase transition driven by deprotonation reaction

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Exchange-correlation kernels in adiabatic-connection fluctuationdissipation DFT – the renormalized ALDA and other kernels from the electron gas

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First principle calculation of anharmonic effect on phonon frequency and spectral functions

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Seeding, nucleation and reactivity of alumina/Ni3Al(111) supported metallic nanoclusters: an ab-initio investigation

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Low energy polymorphs of glycine from automated crystal structure prediction including vdW-aware functionals

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Theophylline self-assembled structures on gold surfaces

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Optical nonlinear properties for solids and nanostructures: theory and numerical simulations

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Adsorption of pyridine on graphene

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Spin-Orbit interactions in single layer and nanoribbons of NiSe2

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Thermoelectric properties of AgSbTe2 from first-principles calculations

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Density functional investigation of spin polarization in bulk and thin films of nitrogen intercalated Cu3N

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Feasible and reliable ab initio calculations of materials relevant for nuclear waste management

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Dielectric matrix formulation of correlation energies within the Random Phase Approximation: Inclusion of (screened) exchange effects

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A multi-scale protocol for simulating the optical properties of natural dyes in solution

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Latent heat of magnetization for MnFeSi0.33P0.66

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A real-time DFT scheme for electronic transport

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Exploring a non-local correlation functional: One-electron selfinteraction, potential asymptotics, and localized states

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First-principles based descriptor for intrinsic charge carrier mobility in organic devices

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Blue phosphorene - metal interface study from first principles

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On the orbital ordering transition in KCuF3

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First-principles methods for 2D materials: electron-phonon interaction, strain-induced fields and screening in graphene

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A theoretical analysis of the role of defects and doping in hexagonal boron nitride sheets

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Physical Factors Influencing Excited State Charge Transfer at the Perylene – Titanium Oxide Interface

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Self-Consistent Continuum Solvation model for the optical properties of complex molecular systems in solution

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Spin asymmetric band gap opening in graphene by Fe adsorption

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Modelling Cancellation Effects in the Optical Response of Many-Electron Systems

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Tuning spin transport properties and molecular magnetoresistance through contact geometry

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***Ab initio* study of structural and vibrational properties of energetic solids**

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Protein field effects on electronic excitations of biological chromophores: a QMC and GW/BSE approach in QM/MM environment

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Adsorption and dissociative adsorption of Nitric Oxide (NO) on Rh cluster over MgO(001) surface

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Electron and Optical Spectroscopies of Graphene Nanoribbons on Au(111): Insights from Ab-Initio Calculations

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***Ab-initio* modeling of peroxy bridge defect in amorphous silica**

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Ab-initio studies of geometric and electronic properties of group VI-B transition metal dichalcogenides monolayers

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International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods

15 January 2015 - 17 January 2015
Trieste - ITALY
Psi-k, Consorzio per la Fisica di Trieste, CECAM , SISSA

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