

# **WORKSHOP mini 2012 on**

COMPUTATIONAL CONDENSED  
MATTER PHYSICS, MATERIALS  
SCIENCE and NANOSCIENCE  
from FIRST PRINCIPLES

**BARCELONA, JANUARY 12-14 2012**

**[www.icmab.es/mini2012](http://www.icmab.es/mini2012)**

## SUMMARY

The workshop “Computational Condensed Matter Physics, Materials Science and Nanoscience from First-Principles” (mini2012) was held in Barcelona between the 12th and 14th of January 2012. This workshop was part of the series of “International Workshops on Computational Physics and Materials Science: Total Energy and Force Methods”, which take place at Trieste’s ICTP in odd years and at a different location in even years, the previous one having been in Shanghai in 2010. The workshop had around 90 participants, including invited speakers and members of the International Scientific Committee. We had very lively sessions covering the latest developments in first-principles methods, featuring quantum Monte Carlo techniques, new DFT functionals, and schemes for large scale simulations. The sessions focused on applications covered problems in magnetism and topological phases, electrochemistry and photocatalysis, electron dynamics, strong correlations, as well as miscellaneous topics in material science. The scientific quality of the talks and discussions was very high, and the same applies to the very crowded poster session that we had in the first evening. All in all, we believe the workshop succeeded in providing a broad view of the current state of the field, combined with some topics that are not so well-known to the community at large or to the regular attendees of the series. The activity was evaluated very positively by the International Scientific Committee and regular participants. This opinion is shared by the local organizers, as the workshop exceeded our expectations regarding both its scientific quality and the number and liveliness of the interactions it fostered.

## SCIENTIFIC CONTENT AND DISCUSSIONS

The scientific content of the workshop revolved around the latest developments in first-principles electronic structure theory, and more generally on the application of cutting-edge numerical methods in nanoscience, condensed matter physics and materials science. The workshop was organized in a number of invited oral sessions, where internationally recognized experts were called to present what we judged to be the most significant advances of the past few years. While the specific topics of each session were diversified to offer a reliable snapshot of the current status of the field, there were some recurrent themes that characterized most of the oral presentations, namely: I) the reliable description of electron correlations, II) strategies to overcome the stringent time- and length-scale limitations of DFT, III) electron excitations, ultrafast dynamics and non-adiabatic processes; IV) magnetism and novel materials characterized by non-trivial band topologies. With the partial exception maybe of the last point (topological insulators are a class of materials where the most peculiar aspects of the physics can often be captured already at the single-particle level) these are the most outstanding and difficult challenges that the field is facing, and all the speakers did an excellent job at portraying the serious efforts that are being made worldwide, in order to make significant progress along these crucial methodological issues. Some of the sessions were more oriented towards applications, but nonetheless followed the traditional style of this series of conferences and workshops: dealing with systems or phenomena that are “difficult” to describe within standard density functional theory, and that require special care to cope, e.g. with quantum nuclear fluctuations in ice (M. Fernandez-Serra), or with the complexity of transition-metal oxides (J. Junquera, J. Kunes, T. Saha-Dasgupta). Most of the oral presentations generated lively discussions, demonstrating once more the novelty of the topics, which are not fully established within the community yet. Overall, we have the feeling that the theory sessions (e.g. on Quantum Monte Carlo, DFT Functionals, Electron Dynamics) were characterized by especially insightful debates, that we

believe have produced a constructive and fruitful exchange of ideas between the participants. Alongside the oral sessions, there was also a poster session where all participants were encouraged to present their results. At the end of the first day, after so many oral talks, we were pleasantly surprised to see that the participants weren't tired or intimidated by the sheer amount of information they were exposed to, and got involved into many discussions, thus contributing to a lively and successful poster session. In the poster session we were also pleased to see a large participation of young scientists working locally in Barcelona, and more generally in Spain. One of the motivations behind the "MINI" series of workshops is to give a marked priority to participants coming from the Country where the workshop is hosted. Also from this point of view, we can say that the workshop fulfilled our aims, and more generally the guidelines of the International Steering committee. All in all, the scientific contents of the workshop were in line with the tradition of high quality and attention to the cutting-edge developments that has characterized the "MINI" series throughout the years. At the same time, we succeeded at keeping a balance between formal theory and applications, so that the sessions could appeal to a broader audience. The encouragingly warm response, both from the scientific committee and by the regular participants, clearly confirmed this success.

## RESULTS AND IMPACT FOR FUTURE DIRECTIONS OF THE FIELD

Given the extraordinarily high quality, diversity and interest of the presentations, it is impossible to discuss here the many ways in which this workshop may affect the scientific development of the field and the future work of their participants. Nevertheless, we believe some broadly-shared impressions can be highlighted.

The quantum Monte Carlo (QMC) session was impressive for the quality of the methodological developments that were presented. Also, and maybe more interestingly, it reflected the momentous stage of the field, the current goal being to popularize QMC methods so that they become a mainstream tool inside the community, hence the proclaimed goal of producing QMC programs that can be used as a “black box”. The situation for QMC was thus presented as comparable to that of DFT methods about 15 or 20 years ago; if this gets confirmed, it could change the way many difficult problems are treated in our community, as QMC could come as a very welcome tool for, at the very least, producing benchmark results to measure the accuracy of (or fit) other simpler approaches. At any rate, it is clear that QMC will be attracting renewed attention and efforts in coming years, and that many workers in the community will be paying a lot of attention to its evolution.

Another approach that attracted great interest was density matrix functional theory (DMFT), especially in what regards its application to magnetic systems. This issue led to very lively discussions during the workshop and, at a minimum, the conclusions are that (1) there is an urgent need to develop DMFT in this area and (2) there is a language breach that needs to be closed between DMFT experts and workers on applications of first-principles methods to magnetic problems (e.g., to strongly-correlated-electron systems). We think the workshop was very effective in evidencing these issues and motivating the community to take action about them in the near future.

The new methods for accurate time-dependent density functional theory (TDDFT) simulations of solids were an eye-opener for many participants of the workshop. The presentations on the topic received great interest, and the urgent need to further develop and popularize such methodologies was made clear. Again, we think the workshop was very effective in bringing together the developers of new methods and the (large) community of potential users, which we think guarantees effective and increased activity along these lines in the future.

Finally, the short but intense session on large scale simulations featured various elegant and suggestive approaches for both hybrid (system-embedding based) and full *ab initio* simulations of very big systems. The spectacular results presented by both speakers (J. Neugebauer and J. VandeVondele) constituted strong motivation for other code developers to implement/improve the new schemes, which should lead to their desirable generalization and application to a variety of (probably more challenging) problems. Here again, we think our workshop served its purpose and will contribute to shape much future activity in the field.

## Scientific Program

Thursday, January 12<sup>th</sup>, 2012

### Morning

08:30 REGISTRATION

08:50 OPENING REMARKS

09:00-11:00 SESSION: **Quantum Monte Carlo** - Chair: Claudia Filippi (U. Twente)

09:00 **Ali Alavi** (University of Cambridge, UK)  
*Quantum Monte Carlo approach to the full CI problem: recent progress*

09:40 **Sandro Sorella** (SISSA, Italy)  
*Efficient Resonance Valence Bond approach for electronic structure*

10:20 **Shiwei Zhang** (College of William and Mary, USA)  
*Recent progress in electronic structure calculations by auxiliary-field quantum Monte Carlo*

11:00-11:30 COFFEE BREAK

11:30-12:50 SESSION: **Materials I** - Chair: Nicola Marzari (EPFL)

11:30 **Mariví Fernandez-Serra** (Stony Brook University, USA)  
*Anomalous Nuclear Quantum Effects in Ice*

12:10 **Javier Junquera** (Universidad de Cantabria, Spain)  
*Highly-confined spin-polarized two-dimensional electron gas in SrTiO<sub>3</sub>/SrRuO<sub>3</sub>*

13:00-15:00 LUNCH BREAK

### Afternoon

15:00-17:00 SESSION: **Magnetism and Topological Phases** - Chair: David Vanderbilt (Rutgers)

15:00 **Stefan Blügel** (Jülich Forschungszentrum, Germany)  
*Spin relaxation mechanisms in metallic systems: Resonance and anisotropy effects*

15:40 **Ivo Souza** (Universidad del País Vasco, Spain)  
*Wannier-based description of orbital magnetic effects in ferromagnets*

16:20 **Oleg Yazyev** (EPFL, Switzerland)  
*Bismuth chalcogenide topological insulators from first principles*

17:00-19:00 COFFEE BREAK & POSTER SESSION

Friday, January 13<sup>th</sup>, 2012

## Morning

09:00-11:00 SESSION: **New DFT Functionals** - Chair: Lucia Reining (École Polytechnique)

- 09:00 **Sangeeta Sharma** (Max Planck Halle, Germany)  
*Treatment of strongly correlated systems within the framework of reduced density matrix functional theory*
- 09:40 **Gustavo E. Scuseria** (Rice University, USA)  
*Symmetry breaking and restoration in electronic structure theory*
- 10:20 **Andreas Savin** (Université Pierre et Marie Curie, France)  
*Coupling wave function with density functional calculations*

11:00-11:30 COFFEE BREAK

11:30-12:50 SESSION: **Electrochem. & Photocatalysis** - Chair: Shobhana Narasimhan (JNCASR)

- 11:30 **Annabella Selloni** (Princeton University, USA)  
*First principles simulations of materials and processes in photo- and electro-catalysis*
- 12:10 **Michiel Sprik** (University of Cambridge, UK)  
*Reactivity of holes at the TiO<sub>2</sub>/water interface*

13:00-15:00 LUNCH BREAK

## Afternoon

15:00-17:00 SESSION: **Electron Dynamics** - Chair: Steven G. Louie (UC Berkeley)

- 15:00 **Matteo Gatti** (Universidad del País Vasco, Spain)  
*Design of effective kernels for spectroscopy: time-dependent current-density-functional theory*
- 15:40 **Fernando Martín** (Universidad Autónoma de Madrid, Spain)  
*XUV/X-ray femto- and attosecond laser pulses for ultrafast electronic control in simple molecules: towards attochemistry?*
- 16:20 **Marco Schirò** (Princeton University, USA)  
*Dynamics of Strongly Correlated Electrons out of Equilibrium*

17:00-17:30 COFFEE BREAK

17:30-18:50 SESSION: **Large Scale Simulations** - Chair: Richard M. Martin (U. of Illinois)

- 17:30 **Johannes Neugebauer** (TU Braunschweig, Germany)  
*Subsystem-Based Time-Dependent Density-Functional Theory for Biomolecular Spectroscopy*
- 18:10 **Joost VandeVondele** (University of Zürich, Switzerland)  
*Simulating large condensed phase systems with GGA and hybrid density functionals*

## Evening

20:30 CONFERENCE DINNER

Saturday, January 14<sup>th</sup>, 2012



## Morning

09:00-11:00 SESSION: **Materials II** - Chair: Xingao Gong (Fudan U.)

09:00 **Jörg Neugebauer** (Max Planck Düsseldorf, Germany)  
*Fully ab initio determination of free energies: Application to modern high-strength steels*

09:40 **Cheol-Hwan Park** (Massachusetts Institute of Technology, USA)  
*Many-body effects on the carrier dynamics of graphene*

10:20 **Rubén Pérez** (Universidad Autónoma de Madrid, Spain)  
*Probing nanostructures with forces and currents*

11:00-11:30 COFFEE BREAK

11:30-12:50 SESSION: **Strong Correlations** - Chair: Eric Koch (Jülich)

11:30 **Jan Kuneš** (Academy of Sciences, Czech Republic)  
*Thermal and doping effects in materials with competing multiplets*

12:10 **Tanusri Saha Dasgupta** (SN Bose Centre for Basic Sciences, India)  
*A Realistic Theory of Correlated Oxides*

12:50 CLOSING REMARKS

13:00-15:00 LUNCH

## PARTICIPANTS

### Invited Speakers

Andreas Savin, Universite Pierre et Marie Curie, France  
Gustavo E. Scuseria, Rice University, USA  
Sangeeta Sharma, Max Planck Halle, Germany  
Ali Alavi, University of Cambridge, UK  
Sandro Sorella, SISSA, Italy  
Shiwei Zhang, College of William and Mary, USA  
Stefan Blügel, Jülich Forschungszentrum, Germany  
Ivo Souza, Universidad del País Vasco, Spain  
Oleg Yazyev, EPFL, Switzerland  
Jan Kunes, Academy of Sciences, Czech Republic  
Tanusri Saha Dasgupta, SN Bose National Centre for Basic Sciences, India  
Matteo Gatti, Universidad del Pais Vasco, Spain  
Fernando Martin, Universidad Autonoma de Madrid, Spain  
Marco Schiro, Princeton University, USA  
Annabella Selloni, Princeton University, USA  
Michiel Sprik, University of Cambridge, UK  
Marivi Fernandez-Serra, Stony Brook University, USA  
Javier Junquera, Universidad de Cantabria, Spain  
Jorg Neugebauer, Max Planck Dusseldorf, Germany  
Cheol Hwan Park, Massachusetts Institute of Technology, USA  
Ruben Perez, Universidad Autonoma de Madrid, Spain  
Johaness Neugebauer, Technical University Braunschweig, Germany  
Joost VandeVondele, University of Zurich, Switzerland

### Scientific Committee (attending the workshop)

Stefano Baroni, SISSA - Trieste, Italy  
Claudia Filippi, Univ. Twente, Netherlands  
Xingao Gong, Fudan University, China  
Francesco Mauri, Univ. Pierre et Marie Curie, France  
Erik Koch, Forschungszentrum Jülich, Germany  
Steven G. Louie, Univ. California - Berkeley, USA  
Richard M. Martin, University of Illinois, USA  
Nicola Marzari, EPFL, Switzerland  
Shobhana Narasimhan, JNCASR - Bangalore, India  
Lucia Reining, École Polytechnique - Paris, France  
David Vanderbilt, Rutgers University, USA

## Organizing Committee (attending the workshop)

Pablo Ordejón, CIN2, Spain

Jorge Iñiguez, ICMAB, Spain

Massimiliano Stengel, ICMAB, Spain

Daniel Sanchez-Portal, Centro de Física de Materiales, Spain

## Other participants

Hideaki Sawada, Nippon Steel Corporation, JAPAN

Josep María Oliva, Instituto Rocasolano - CSIC, Spain

Alberto Marmodoro, Max-Planck-Institut für Mikrostrukturphysik, Germany

Jose María Soler, Universidad Autónoma de Madrid, Spain

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Nicolai A. Bogdanov, Inst. Theoretical Solid State Physics - Dresden, Germany

David Soriano, ICN, Spain

P. Andre Clayborne, University of Jyväskylä, Finland

Perla Wahnón, UPM, Spain

Diego Carrascal, Univ. Oviedo, Spain

Gian-Giacomo Asara, U. Rovira i Virgili, Spain

Christina Ebensperger, University Erlangen-Nürnberg, Germany

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**ABSTRACTS**  
INVITED TALKS

## I-1

### Quantum Monte Carlo Approach to the Full CI Problem: Recent Progress

A. Alavi

*University of Cambridge, UK*

The ground-state eigenvalue problem posed by the electronic Schrödinger equation can be cast as a stochastic process involving an annihilating population of positive and negative walkers that inhabit Slater determinant space [1]. The population of walkers evolve according to a simple set of rules, which are derived from the underlying imaginary-time Schrödinger equation, such that the long-time distribution of the walkers matches the exact ground-state eigenvector. We show that this algorithm has a remarkable emergence characteristic, akin to symmetry-breaking phase transitions in classical statistical mechanical systems.

The use of Slater determinants obviates the usual Fermion sign problem of diffusion Monte Carlo (namely the collapse onto Bosonic wavefunctions), but instead introduces a different sign problem associated the fact that the off-diagonal Hamiltonian matrix elements are both positive and negative. This sign problem however can be solved through a combination of walker annihilation and a "survival of the fittest" criterion [2] (the latter greatly reducing the dependence of the algorithm on walker annihilation). The method provides a way to compute exact electronic energies within a specified N-electron basis set. We will give examples of the algorithm at work in real systems in sizeable basis sets, ranging from atomic electron affinities, and dissociation energies of diatomic molecules. Recent progress on the application of the method to compute density matrices will also be presented.

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

[2] Deidre Cleland, G.H. Booth, and Ali Alavi, J. Chem. Phys., 132, 041103, (2010).

[3] Deidre Cleland, George Booth, and Ali Alavi, J. Chem. Phys., 134 , 024112, (2011)

**I-2**

## **Superconductivity from Strong Electron Correlation: from the Hubbard Model to Graphene and High Tc Materials**

S. Sorella

*SISSA - Scuola Internazionale Superiore di Studi Avanzati, Trieste, Italy*

We report novel ab initio simulations based on an highly correlated variational wave function, able to describe High-Tc superconductivity without the conventional phonon mediated mechanism. By means of a variational approach based on the quantum Monte Carlo method the pairing function and its symmetry is determined fully ab-initio by total energy minimization. It is found that in graphene, the pairing function has an extended s-wave symmetry and becomes very small for large number of Carbon atoms. Preliminary results are presented also for parent compound cuprate superconductors and pnictides.

### I-3

## Recent Progress in Electronic Structure Calculations by Auxiliary-field Quantum Monte Carlo

Shiwei Zhang

*College of William and Mary, USA*

Recent progress has advanced the auxiliary-field quantum Monte Carlo (AFQMC) method considerably towards a general approach for *ab initio* many-body total energy calculations of materials and realistic models. This method uses importance-sampled random walks in the space of Slater determinants to project out the many-body ground state, or excited state. A constraint on the overall phase of the Slater determinant is applied to remove the sign problem. The approximation can be systematically improved at the cost of additional computing (releasing the constraint) or better constraining trial wave functions. I will discuss applications in the accurate determination of structural and magnetic properties, and calculations of excited states, in both quantum chemistry and solid state.



## I-4

### Anomalous Nuclear Quantum Effects in Ice

Marivi Fernandez-Serra,<sup>1</sup> P.B. Allen,<sup>1</sup> C. P. Herrero,<sup>2</sup> B. Pamuk,<sup>1</sup> R. Ramirez,<sup>2</sup> J. M. Soler,<sup>3</sup> P. Stephens<sup>1</sup>

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The experimental volume of H<sub>2</sub>O ice is smaller than that of D<sub>2</sub>O, and this isotope shift, with anomalous sign, is not reproduced by state of art empirical potentials.

We show that *ab initio* density functional theory does reproduce it, accounting correctly for a subtle interplay between intermolecular libration modes, with a normal isotope effect, and intramolecular stretching modes. The latter have an anomalous negative quantum effect on the volume, because of the well known anticorrelation between the lengths of the covalent and hydrogen OH--O bonds.

We also show, both experimentally and theoretically that the volume's isotope shift of H<sub>2</sub><sup>18</sup>O ice has positive sign. Relative to the the classical result, the net effect of quantum nuclei (H and O) on volume has the conventional (positive) sign at T=0 but it becomes negative above 70 K, indicating that it may be also relevant for liquid water.

Overall, nuclear quantum effects on the volume of ice are of the order of 1%, indicating that comparisons between classical calculations and experimental lattice constants are misleading. These qualitative conclusions are independent of the exchange and correlation density functional used. However, the quantitative agreement with experiments is a good test for the ability of current exchange and correlation functionals to describe ice and, by extension, liquid water. An analysis of the performance of different density functionals, with and without van der Waals correlations, will be presented.

**Highly-Confined Spin-Polarized Two-Dimensional Electron Gas in SrTiO<sub>3</sub>/SrRuO<sub>3</sub> Superlattices**

J. Junquera,<sup>1</sup> P. García-Fernández,<sup>1</sup> Marcos Verissimo-Alves,<sup>1</sup> Daniel I. Bilc,<sup>2</sup> and Philippe Ghosez<sup>2</sup>

<sup>1</sup>*Departamento de Ciencias de la Tierra y Física de la Materia Condensada, Universidad de Cantabria, Cantabria Campus Internacional, Avenida de los Castros s/n, 39005, Santander, Spain*

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We report first principles characterization of the structural and electronic properties of (SrTiO<sub>3</sub>)<sub>5</sub>/(SrRuO<sub>3</sub>)<sub>1</sub> superlattices. We show that the system exhibits a spin-polarized two-dimensional electron gas extremely confined to the 4*d* orbitals of Ru in the SrRuO<sub>3</sub> layer. Every interface in the superlattice behaves as minority-spin half-metal ferromagnet, with a magnetic moment of  $\mu = 2.0 \mu_B/\text{SrRuO}_3$  unit. The shape of the electronic density of states, half metallicity and magnetism are explained in terms of a simplified tight-binding model, considering only the *t*<sub>2g</sub> orbitals plus (i) the bi-dimensionality of the system, and (ii) strong electron correlations.

## Spin Relaxation Mechanisms in Metallic Systems: Resonance and Anisotropy Effects

Stefan Blügel, Swantje Heers, Nguyen H. Long, Bernd Zimmermann, Yuriy Mokrousov, Rudolf Zeller, Phivos Mavropoulos  
*Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany*

Spin relaxation in non-magnetic materials, i.e. the effect of decay of an out-of-equilibrium spin population of electrons that have been injected into a solid, is of great importance for the functionality and design of spin-electronic devices. In metals with space-inversion symmetry, the main cause for spin relaxation is the Elliott-Yafet mechanism [1, 2], which originates from the combination of electron-scattering processes of any type together with the spin-orbit coupling and the subsequent spin-mixing of the electronic states.

In this contribution we focus on two important aspects of this mechanism. First, we observe that resonant impurity scattering can maximize the spin-flip amplitude, if the Wigner delay time is long enough. The intuitive reason behind this, is, that if an electron stays for a long time at the impurity site before hopping away, then it has enough time to experience the spinorbit interaction due to the nucleus of the impurity and to precess its spin axis accordingly. This means that sharper resonances lead to increased spin-flip amplitudes, which in principle can even reach the unitarity limit.

Second, we analyze anisotropy effects due to the band structure of the host metal. Specifically, in ultra-thin films, but also in non-cubic crystals, we find that the relaxation rate can strongly depend on the spin direction of the injected electrons with respect to the crystallographic axes. The effect originates from the anisotropy of the spin-mixing part of the wave functions on the Fermi surface.

Our calculations are based on density-functional theory for the electronic structure and Fermi-surface properties and on the solution of the multiple-scattering equations for the spin-flip scattering amplitude within the Korringa-Kohn-Rostoker Green function method [3] in which the spin-orbit interaction has been implemented.

This work was supported in part by the Young Investigators Group Programme of the Helmholtz Association (HGF), contract *Topological Nanoelectronics* VH-NG-513 and from the German Science Foundation (DFG) under grant number MO 1731/3-1.

[1] R.J. Elliott, Phys. Rev. 96, 266 (1954)

[2] Y. Yafet, in Solid State Physics, Vol. 14, edited by F. Seitz and D. Turnbull (Academic, New York, 1963), p.2.

[3] N. Papanikolaou, R. Zeller, P. H. Dederichs, J. Phys.: Condens. Matter 14, 2799 (2002).

**Wannier-based Description of Orbital Magnetic Effects in Ferromagnets**Ivo Souza*Universidad del País Vasco, San Sebastián, Spain*

I will discuss the use of Wannier functions (WFs) to calculate two basic quantities in spin-orbit-coupled ferromagnets: the anomalous Hall conductivity (AHC) and the spontaneous orbital magnetization. Both can be expressed as integrals over the Fermi sea: of the Berry curvature for the former, and of a related, but more complex object, for latter. These quantities display strong and rapid variations in  $k$ -space, demanding very dense integration meshes.

By working in the representation of WFs spanning the valence and low-lying conduction bands, it becomes possible to evaluate quickly and accurately the required quantities across the BZ, in the spirit of Slater-Koster interpolation. This "Wannier interpolation" scheme circumvents the need to treat the integration mesh directly from first-principles, with considerable savings in computer time (the WFs themselves can be generated from an *ab initio* calculation on a relatively coarse  $k$ -point mesh). Results will be presented for the transition metals Fe, Co, and Ni, and for the ordered ferromagnetic alloys FePt and FePd.

Oleg Yazyev

*Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland*

Topological insulators are the recently discovered electronic materials that have a bulk electronic band gap, but also exhibit metallic surface states as a consequence of the non-trivial topology of the bulk electronic wavefunctions induced by strong spin-orbit interactions [1,2]. These metallic surface states are characterized by the helical spin textures and the absence of spin degeneracy which makes them immune to scattering and promises novel technological applications. In my talk, I will cover our recent work aiming towards the understanding of basic electronic properties of bismuth chalcogenides  $\text{Bi}_2\text{Se}_3$  and  $\text{Bi}_2\text{Te}_3$ , the reference topological insulators discovered in 2009 [3,4], by means of first-principles calculations. In particular, I will focus on band dispersion and spin textures of the topologically protected surface states in these materials [5]. Exceptionally strong spin-orbit interaction in these materials entangles the electronic states across broad energy ranges thus reducing the spin-polarization of the topologically protected surface states to  $\sim 50\%$ . The helical character of the surface-state charge carriers can be used for controlling the magnitude of spin polarization associated with a charge current in thin films of topological insulators by means of an external electric field. Then, I will cover our recent investigation of  $\text{Bi}_2\text{Se}_3$  and  $\text{Bi}_2\text{Te}_3$  using the highly accurate first-principles many-body perturbation theory based on the *GW* approximation [6]. The quasiparticle self-energy corrections introduce significant changes to the bulk band structures, surprisingly leading to a decrease in the direct band gaps in the band-inversion regime as opposed to the usual situation without band inversion. The introduction of selfenergy corrections in slab-model calculations results in significant shifts of the surface-state Dirac point energies relative to the bulk bands and in enlarged gap openings from the interactions between the surface states across the thin slab, both in agreement with experimental data.

- [1] M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. **82**, 3045 (2010).
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- [5] O. V. Yazyev, J. E. Moore, and S. G. Louie, Phys. Rev. Lett. **105**, 266806 (2010).
- [6] O. V. Yazyev, E. Kioupakis, J. E. Moore, and S. G. Louie, arXiv:1108.2088.

## Treatment of Strongly Correlated Systems within the Framework of Reduced Density Matrix Functional Theory

Sangeeta Sharma, J. K. Dewhurst and E. K. U. Gross

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One of the most dramatic failures of the usual local density approximation or generalized gradient type approximations to the exchange-correlation functional of density functional theory is the incorrect prediction of a metallic ground state for the strongly correlated Mott insulators, of which transition metal oxides (TMOs) may be considered as prototypical. In the present work we extend reduced density matrix functional theory (RDMFT) to the case of solid-state systems and introduce a new functional for their accurate treatment [1]. Furthermore, a method for calculating the spectrum of extended solids within RDMFT is presented. An application of this method to the strongly correlated TMOs demonstrates that (i) an insulating state is found in the absence of magnetic order and, in addition, (ii) the interplay between the charge transfer and Mott-Hubbard correlation is correctly described. In this respect we find that while NiO has a strong charge transfer character to the electronic gap, with substantial hybridization between  $t_{2g}$  and oxygen- $p$  states in the lower Hubbard band, for MnO this is almost entirely absent. As a validation of our method we also calculate the spectra for a variety of weakly correlated materials, finding good agreement with experiment and other techniques [2].

[1] S. Sharma, J. K. Dewhurst, N. N. Lathiotakis and E. K. U. Gross Phys. Rev. B 78, 201103 Rapid Comm. (2008)

[2] S. Sharma, S. Shallcross, J. K. Dewhurst and E. K. U. Gross cond-mat/0912.1118

## I-10

### Symmetry Breaking and Restoration

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We have derived and implemented symmetry-projected Hartree-Fock-Bogoliubov (HFB) equations and apply them to the molecular electronic structure problem. All symmetries (particle number, spin, spatial, and complex conjugation) are deliberately broken and restored in a self-consistent variation-after-projection approach. We show that the resulting method yields a comprehensive black-box treatment of static correlation with effective one-electron (mean-field) computational cost. The ensuing wave function is of multireference character and permeates the entire Hilbert space of the problem. The energy expression is an independent quasiparticle density matrix functional. All reduced density matrices are expressible as an integration of transition one-particle density matrices over a gauge grid. I will present several proof-of-principle examples demonstrating the compelling power of this new method for electronic structure theory [1].

[1] Projected Quasiparticle Theory for Molecular Electronic Structure, G. E. Scuseria, C. A. Jimenez-Hoyos, T. M. Henderson, J. K. Ellis, and K. Samanta, *J. Chem. Phys.* **135**, 124108 (2011).

## I-11

### **Coupling wave function with density functional calculations**

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Already the Kohn-Sham method can be seen as a coupling of a wave function with density functional method: the Kohn-Sham determinant is obtained for a model system, and a density functional is used to correct the energy of the model system to obtain that of the physical system.

In the same way, other Hamiltonians can be defined as model systems. A guide through the possible choices of such Hamiltonians is presented. Among the presently available ones, range separation has merged out as a viable route.



## I-12

### The Interactions of Water and Oxygen with Anatase $\text{TiO}_2$

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The interactions of  $\text{TiO}_2$  with water and molecular oxygen play a key role in the photocatalytic reactions occurring on the surfaces of this material. This talk will cover results of recent density functional theory calculations on the adsorption of water and  $\text{O}_2$  on reduced anatase (101). Anatase is the form of  $\text{TiO}_2$  that is present in most technical nanomaterial. At variance with rutile, its intrinsic reducing defects, i.e., O vacancies and Ti interstitials, reside exclusively in subsurface sites. We shall discuss the influence of subsurface defects on water adsorption and dissociation as well as the mechanisms by which these defects can be healed by  $\text{O}_2$  adsorption. Comparison with available experimental results will be also presented.

## I-13

### Reactivity of Holes at the Titania Water Interface

Jun Cheng,<sup>1</sup> Marialore Sulpizi,<sup>1,2</sup> Joost VandeVondele<sup>3</sup> and Michiel Sprik<sup>1</sup>

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<sup>2</sup>*Department of Physics, Mainz University, Germany*

<sup>3</sup>*Department of Materials, ETH, Zurich, Switzerland*

Holes created by photoexcitation in solid  $\text{TiO}_2$  quickly localize on a small number of oxygen atoms. In this talk we look in detail at the energetics of the reaction of such self trapped holes with surface hydroxide anions left by acid dissociation of adsorbed water molecules. This is the key process in the formation of reactive surface radicals when aqueous  $\text{TiO}_2$  is exposed to light. Electronic energy levels

at the interface are aligned using a recently developed molecular dynamics normal hydrogen electrode [1,2]. Application to holes in metal oxides has become possible only recently thanks to the development of schemes for efficient implementation of hybrid exact exchange functionals for periodic models of extended systems [3].

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[2] F. Costanzo, M. Sulpizi, R. G. della Valle and M. Sprik, J. Chem. Phys. 134 (2011), 244508.

[3] M. Guidon, J. Hutter and J. VandeVondele, J. Chem. Theory Comput. 6 (2010), 2348.

## I-14

### Design of Effective Potentials and Kernels for Spectroscopy: Time-Dependent Current-Density-Functional Theory

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Density-functional theory is an in principle exact theory for the calculation of ground-state properties. However, Kohn-Sham eigenvalues cannot be used to interpret spectra that involve electronic excitations. Today, a successful approach for the calculation of spectral and optical properties in solids is based on many-body Green's-function theory. The bottleneck is that measurable spectra are obtained as contractions of Green's functions. One thus calculates more information than needed. I will show how a generalisation of the Sham-Schlüter equation provides a powerful tool in the design of new efficient computational schemes [1]. As application of this general approach, I will discuss the example of the time-dependent current-density-functional theory [2] and the introduction of a real, local and frequency-dependent effective potential for the calculation of photoemission spectra.

[1] M. Gatti, V. Olevano, L. Reining, and I.V. Tokatly, Phys. Rev. Lett. **99**, 057401 (2007).

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I-15

## XUV/X-ray Femto- and Attosecond Laser Pulses for Ultrafast Electronic Control in Simple Molecules: Towards Attochemistry?

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The development of attosecond laser pulses allows one to probe the inner working of atoms and molecules on the timescale of the electronic response. In molecules, attosecond pump-probe spectroscopy enables investigations of the prompt charge redistribution and localization that accompany photo-excitation processes, where a molecule is lifted from the ground Born-Oppenheimer potential energy surface to one or more excited surfaces, and where subsequent photochemistry evolves on femtosecond timescales. In this talk I will present a few theoretical examples of realistic molecularattosecond pump-probe experiments in which H<sub>2</sub> is ionized with a single attosecondpulse (or a train of attosecond pulses) and is subsequently probed by one or severalinfrared few-cycle pulses. The localization of the electronic charge distribution within the remaining molecular ion is calculated with attosecond time-resolution and isvisualized by varying the delay between the pump and probe pulses. The results of these calculations [1,2] are compared with recent experimental measurements and provide the different mechanisms that are responsible for the observations. Recent advances for more complicated molecules, such as N<sub>2</sub>, CO [3], CH<sub>4</sub> and C<sub>2</sub>H<sub>2</sub> are also reported.

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[3] S. E. Canton, E. Plésiat, J. D. Bozek, B. S. Rude, P. Decleva, and F. Martín "Direct observation of Cohen-Fano interferences in vibrationally resolved valence-shell photoionization spectra of H<sub>2</sub>, N<sub>2</sub> and CO". *Proceedings of the National Academy of Sciences* **108** 7302 (2011)

**Dynamics of Strongly Correlated Electrons out of Equilibrium**

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The non equilibrium dynamics of strongly correlated electronic systems represents a frontier of modern condensed matter physics with applications ranging from pump probe experiments in correlated materials, to non linear transport in correlated nanostructures up to dynamics in ultracold atomic gases. The theoretical description of this physics poses novel conceptual challenges and requires the development of new methods to treat non equilibrium effects and strong correlations on the same footing. Here we present results on the out of equilibrium real time dynamics of a paradigmatic strongly correlated model system, the single band Hubbard model, obtained using novel methods to describe electrons out of equilibrium which include the time dependent Gutzwiller variational approach as well as a non equilibrium extension of Dynamical Mean Field Theory.

**I-17**

## **Subsystem-Based Time-Dependent Density-Functional Theory for Biomolecular Spectroscopy**

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Theoretical spectroscopy of chromophores in biological systems is often complicated by the necessity to accurately represent environmental effects [1]. In particular polarization effects due to the surrounding medium (e.g., protein matrix, solvent) and exciton couplings in protein-pigment complexes are a challenge for electronic-structure methods, which often require the use of parametrized hybrid and/or effective Hamiltonian models.

Here, new developments and applications within the subsystem-based time-dependent density functional theory (subsystem TDDFT) [2] for the inclusion of environmental response effects will be discussed, and a comparison to QM/MM methods employing polarizable classical force fields will be made. It will be outlined how different types of polarization effects can be distinguished in the formalism. Applications of subsystem TDDFT to the excited states and electronic spectra of protein-pigment complexes like the photosynthetic light-harvesting complex LHC-II [3] will be presented.

[1] J. Neugebauer, ChemPhysChem 10 (2009), 3148.

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I-18

## Simulating Large Condensed Phase Systems with GGA and Hybrid Density Functionals

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Traditionally, *ab initio* molecular dynamics (AIMD) of condensed phase systems is performed using local density functionals (GGAs). The use of GGAs allows for MD simulations containing a thousand atoms, and static calculations on systems containing millions of atoms. Hybrid functionals, which include a non-local component such as Hartree-Fock exchange, remained prohibitively expensive until recently. Here, we present a linear scaling approach to hybrid DFT that is suitable for condensed phase MD simulations. The approach is based on the use of a truncated Coulomb operator. A massively parallel implementation allows AIMD simulations to be performed with good time to solution. Furthermore, a new approximation to Hartree-Fock exchange will be presented that allows for a significant reduction in computational cost using an approximate density matrix method (ADMM). ADMM exploits the fact that Hartree-Fock exchange can be evaluated rapidly for systems with small basis sets or sparse density matrices, and uses an exchange functional to correct for the difference between the approximate and exact density matrix. This approach captures the most important features of hybrid functionals, such as an improved band gap and reduced self interaction error, while it is similar to a GGA calculation in cost.

Guidon M; Hutter J; VandeVondele J; 2010

Auxiliary density matrix methods for Hartree-Fock exchange calculations.

[JOURNAL OF CHEMICAL THEORY AND COMPUTATION 6\(8\): 2348-2364](#)

Guidon M; Hutter J; VandeVondele J. 2009

Robust Periodic Hartree-Fock Exchange for Large-Scale Simulations Using Gaussian Basis Sets.

[JOURNAL OF CHEMICAL THEORY AND COMPUTATION 5\(11\): 3010-3021](#)

Guidon, M; Schiffmann, F; Hutter, J; VandeVondele, J. 2008

Ab initio molecular dynamics using hybrid density functionals.

[JOURNAL OF CHEMICAL PHYSICS 128 \(21\): 214104](#)

I-19

## ***Ab initio* Guided Steel Design: Concepts, Prospects and Challenges**

Jörg Neugebauer

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The combination of accurate first principles calculations with thermodynamic and kinetic concepts has quickly advanced in the past few years and allows now to tackle even complex advanced engineering materials. Key to these studies is the accurate determination of thermodynamic properties, with the free energy being the central quantity. In the talk recently developed concepts connecting high convergence densityfunctional theory calculations, new approaches to describe finite temperature magnetism and efficient sampling strategies will be shown to allow an unbiased and accurate determination of all relevant contributions of the free energy. The flexibility and the predictive power of this approach will be discussed for examples relevant to the design and understanding of modern high strength steels and light-weight alloys.



**Many-body effects on the carrier dynamics of graphene**

Cheol-Hwan Park,<sup>1,2,3</sup> Feliciano Giustino,<sup>1,2</sup> Catalin D. Spataru,<sup>4</sup> Marvin L. Cohen,<sup>1</sup> and Steven G. Louie<sup>1</sup>

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In this presentation, I will explain that the measured carrier scattering rate versus energy behavior in graphene can be quantitatively described from first-principles calculations considering electron-electron interactions within the GW approximation and electron-phonon interactions within the Migdal approximation [1]. Then, I will show that such calculations can also explain (i) the mismatch between the extrapolations of the upper and lower Dirac cones in heavily doped graphene [2] and (ii) the significant deviation from linear energy dispersion in extremely low-doped graphene [3]. Electron-electron interactions play a key role in both of these phenomena.

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R. Pérez

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In this talk, we focus on the application of Scanning Tunneling (STM) and Atomic Force Microscopy with atomic resolution (AFM) [1] to carbon nanostructures (graphene, carbon nanotubes and fullerenes) and oxides. The simple honeycomb structure shared by the carbon materials represents both a perfect testing ground and a fundamental challenge for scanning microscopy imaging. STM can achieve atomic resolution in graphite even in ambient conditions but, after 25 years of research, still there is no consensus whether the maxima in the atomic scale images correspond to atoms or to the hollow sites. To tackle this long-standing problem, we have performed complex first-principles calculations of forces and currents between a tip and carbon nanostructures. Our results explain the rich variety of image patterns observed in both AFM and STM experiments in terms of two factors: (i) the tip-sample distance and (ii) the chemical reactivity of the tip [2]. Based on this work, we have explored the electronic properties of epitaxial graphene on metals, both in the case of the pristine layer and in the presence of carbon vacancies, where the calculations help to correlate the structure of the defect with the experimental STM images [3]. These calculations also shed light on the possible magnetic state associated with these defects, predicted but not experimentally confirmed, in graphite [4].

In the case of the oxide surfaces, the investigation of these novel catalysts requires a comprehensive experimental method for the identification and rapid characterization of prospective catalytically active sites. We show how progress in this direction can be achieved by the combination of three-dimensional atomic force microscopy (3D-AFM) [5] with simultaneous STM measurements and our theoretical simulations to study rutile  $\text{TiO}_2(110)$  [6] and the oxygen-terminated copper (100) surfaces [7]. The wealth of site-specific information obtained is promising for future applications, but the interpretation of the wide range of contrast modes requires a thorough characterization of the sources of contrast in AFM and STM imaging. Our force and current calculations provide insight into (1) the tip structures responsible for the different imaging modes and (2) into the correlation between tip-sample forces and local chemical reactivity.

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[3] M. M. Ugeda et al., Phys. Rev. Lett. 107 (2011) 116803

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**Thermal and doping effects in materials with competing multiplets**

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The spectra of an isolated atom consists of multiplets of states, in which a given atom stays forever. The behavior of a weakly correlated metal or covalently bonded insulator is, on the other hand, characterized by fast fluctuations which sample large number of the atomic multiplets. In strongly correlated metals or Mott insulators these fluctuations are strongly suppressed and typically a single multiplet dominates. In some materials, however, several multiplets may happen to be competing. A well known example is  $\text{LaCoO}_3$  in which the lowest non-magnetic singlet is just slightly below a multiplet with a finite total spin. This gives rise to very strong temperature dependencies of many physical quantities, such as magnetic susceptibility, conductivity or bond-lengths. We use the dynamical mean-field theory to investigate these effects. We will present results obtained on a minimal 2-band Hubbard model. We will show that ordered state which breaks the translational symmetry exists in the parameter range of interest and interpret this state using an approximate mapping to the classical Blume-Emery-Griffiths model. We will further present results for the actual  $\text{LaCoO}_3$  obtained within the LDA+DMFT framework. Finally, we will discuss the effect carrier doping which may lead to an unusual behavior such as formation of nanoscopic inhomogeneities.

Jan Kuneš and Vlastimil Křápek, *Phys. Rev. Lett.* **106**, 256401 (2011).

## A Realistic Theory of Correlated Oxides

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Materials like transition metal oxides are characterized with strong electron-electron correlation effects. However, the anomalous properties of these materials are sensitive to small changes in doping, temperature and pressure. This indicates that these properties are the result of a delicate interplay between correlation effects and the chemistry. Understanding of these materials, therefore, demands development of theories that can handle the correlation effect and the material related aspects on the same footing. A significant development made in this context is the application of density functional theory (DFT) based method to capture material dependence in conjunction with Dynamical Mean Field Theory (DMFT) to capture the strong electron-electron correlation. In this talk we will discuss a Wannier function based formulation [1] of such approach. We will focus on application of the developed method to classic problem of  $V_2O_3$  [2], ruthenates [3] and manganites at nanoscale [4].

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# **ABSTRACTS**

## POSTERS

## Electronic Structure of Aluminum Superatom Complexes

P. Andre Clayborne,<sup>1\*</sup> O. Lopez-Acevedo,<sup>1</sup> R. L. Whetten,<sup>1,2</sup> H. Grönbeck,<sup>3</sup> and H. Häkkinen<sup>1,4</sup>

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Metal clusters stabilized by a surface ligand shell represent an interesting intermediate state of matter between molecular metal-ligand complexes and bulk metal. Such clusters are dominated by metal-metal bonds in comparison to the metal-ligand bonds on the exterior of the cluster. The electronic stability of thiolate-protected gold clusters, clusters with a metallic gold core and metallo-organic ligand shell, can be explained as *superatom complexes* analogous to giant atoms based on the electronic shell structure.[1] Using ab-initio computational techniques, we illustrate the *superatom complex model*, with angular momentum shells up to  $L = 6$  symmetry, can be used to explain the electronic stability of ligand-stabilized aluminium clusters.[2-3]

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**P-2**

## **Effective Atomic Pseudopotentials for Large Scale Electronic Structure Calculations**

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We derive a new type of pseudopotentials from conventional norm-conserving pseudopotentials for the treatment of a large number of atoms. These effective pseudopotentials are a one to one mapping of the effective potential obtained from a self-consistent density functional theory (DFT) calculation and are parameter free. The pseudopotentials are not aimed at the calculation of the total energy, but of band edge states relevant for optical processes. The restriction to only band edge states and the lack of self-consistency allows us to reduce the size of the eigenvalue problem significantly, compared to a traditional DFT calculation. We describe the pseudopotential generation and benchmark its quality and transferability by comparison to standard DFT calculations of bulk and quantum wells. In general we obtain agreement within a few tens of meV for quantum well structures. This demonstrates the transferability of the pseudopotentials and a surprising universality of their long-range behavior. We find that our effective pseudopotentials are material dependent (in contrast to ab-initio pseudopotentials that depend on the type of atom only) but are transferable within different structures made from this material. We discuss the generation of accurate pseudopotentials for open surfaces and discuss how self-consistent charge rearrangements must be included.

### P-3

## Electronic Structure of Strongly Correlated Materials with *Ab Initio* Quantum Chemical Methods

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Fully *ab initio* wave-function-based methods from modern quantum chemistry are employed for the study of the electronic structure of Ti  $d^1$ , V  $d^2$  and Cu  $d^9$  correlated systems, in particular, the TiOCl, VOCl, YVO<sub>3</sub> and Ca<sub>2+x</sub>Y<sub>2-x</sub>Cu<sub>5</sub>O<sub>10</sub> compounds. We investigate N-particle excitations as those probed in optical absorption and RIXS (resonant inelastic x-ray scattering) measurements. The strong correlations are treated within the CASSCF (complete-active-space selfconsistent-field) approximation while remaining correlation effects are handled by MRCI (multi-reference configuration-interaction) techniques. Since such correlation calculations can be carried out only for a finite region of the crystal, the remaining part of the solid should be judiciously constructed. We use in these studies an *ab initio* embedding scheme in which the effective embedding potential is constructed on the basis of prior periodic Hartree-Fock calculations for the extended crystal. Results for the *d*-orbital electronic structure of the mentioned compounds are compared with recent experiments.

For TiOCl, the computed *d*-level electronic structure and the symmetries of the wave functions are in very good agreement with RIXS results and optical absorption data. For VOCl, future resonant inelastic x-ray scattering experiments will constitute a direct test of the symmetry and energy of about a dozen of different *d-d* excitations that we predict here. The *ab initio* results we report for Ca<sub>2+x</sub>Y<sub>2-x</sub>Cu<sub>5</sub>O<sub>10</sub> should be helpful for the correct interpretation of RIXS experiments on this highly anisotropic compound.



## P-4

### Electron-Phonon Coupling in Rubrene: A DFT Calculation

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Electronic transport in organic semiconductors is dominated by several factors, with interaction of electrons and phonons being of great importance. The strong electron-phonon interaction taking place in these materials has a much stronger impact on organic semiconductors compared to inorganic ones, as the band widths are much smaller. As a consequence, this interaction implies specific transport characteristics which cannot be described by conventional approaches such as the perturbative calculation of the relaxation time in the Boltzmann equation. In contrast to these conventional approaches, a recently developed charge-transport theory [1,2] that explicitly deals with the influence of the electron-phonon coupling on transport properties in these materials non-perturbatively can describe phonon-induced hopping and band transport on equal footing.

Here, we will present the first ingredients to apply such theory to rubrene, one of the most widely studied organic semiconductors. In particular, we performed Density Functional Theory calculations of the phonon modes and the electron-phonon coupling in rubrene. The calculations are done using the efficient SIESTA code [3], which allows the determination of these properties in crystals with a large number of atoms (as the case of rubrene, which contains 280 atoms in the unit cell). I will describe the results of our calculations, and focus on the phonon modes that have a stronger impact on the highest valence band, which are the relevant states for hole conduction. I will also describe work aimed at extracting a simplified model which contains the essential aspects of the electronic states of the hole band and the influence of the phonons, which will be later used to determine the transport properties using the methodology proposed in Ref. [1].

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**P-5**

## **Exact Kohn-Sham Eigenstates versus Quasi-Particles in Simple Models of Strongly Correlated Electrons**

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We present analytic expressions for the exact density functional and Kohn-Sham Hamiltonian of simple tightbinding models of correlated electrons. These are the single- and double-site versions of the Anderson, Hubbard and spinless fermion models. The exact exchange and correlation potentials are fully non-local. The analytic expressions allow to compare the Kohn-Sham eigenstates of exact density functional theory with the many-body quasi-particle states of these correlated-electron systems. The exact Kohn-Sham spectrum describes correctly many of the non-trivial features of the many-body quasi-particle spectrum, as for example the precursors of the Kondo peak. However, we find that some pieces of the quasi-particle spectrum are missing because the many-body phase-space for electron and hole excitations is richer.

## P-6

### First-Principles Modeling of Pt/LaAlO<sub>3</sub>/SrTiO<sub>3</sub> Nanocapacitors under an External Bias Potential

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We study the electronic, structural and electrical properties of Pt/LaAlO<sub>3</sub>/SrTiO<sub>3</sub> nanocapacitors under the action of an external applied bias, using first-principles calculations performed at fixed electric displacement  $D$  [1]. In particular, we deduce a complete set of *ab initio* band diagrams and a simple analytical expression for the electric field within LaAlO<sub>3</sub> (LAO) as a function of film thickness and the applied bias potential. In addition, we investigate the capacitance of the metal-oxide heterostructure in a field-effect transistor setup. We find that the electric field within LAO is a non-intrinsic quantity that monotonically decreases with increasing the LAO thickness. The occurrence of spontaneous Zener tunneling in this system, therefore, is ruled out. We also find that, while the Pt electrode behaves almost ideally (i.e. provides perfect charge screening), the LAO/STO interface is associated with a capacitance, predominantly due to band bending effects, that is constant within a wide range of carrier densities. We discuss the implications of our results in the light of recent experimental observations on biased LAO/STO junctions with metallic top electrodes [2,3].

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## **P-7**

### **Electronic Structures of Antiferromagnetic BaFe<sub>2</sub>As<sub>2</sub>**

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In quasi one- and two-dimensional metals the electrons can be organized into regular patterns, and this phenomenon is known to be the charge-density wave (CDW) or spin-density wave (SDW). The parent compound of iron-based superconductors, BaFe<sub>2</sub>As<sub>2</sub>, undergoes both structural and magnetic phase transitions. The crystal structure changes from tetragonal to orthorhombic and the magnetic ground state changes from paramagnetic to antiferromagnetic at about 140 K. SDW anomaly at 140 K, which is believed to be an important prerequisite for high-T<sub>c</sub> superconductivity in iron-based superconductors, was also observed.

We performed the first-principles calculation for the BaFe<sub>2</sub>As<sub>2</sub> compound in various antiferromagnetic states, and the electronic structures and Fermi surface are carefully investigated. While there have been considerable debates as to whether the antiferromagnetism is due to the Fermi surface nesting or to second neighbor superexchange, through our results, we can deduce the correlation between the SDW (&CDW) and the Fermi-surface nesting.

## **P-8**

### **First-Principles Investigation of Phase-Change Effects in Multiferroics**

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Using first-principles calculations we have characterized new phases of bulk multiferroic materials that are close in energy to the ground state, but that display very different properties. This suggests that the application of electric fields could induce phase changes that would involve large effects of different kinds. In particular, (i) we have found stable supertetragonal bulk phases for the prototype multiferroic bismuth ferrite [Diéguez et al., Phys. Rev. B 83, 094105 (2011)], and (ii) we propose to use a solid solution of bismuth ferrite and bismuth cobaltite to create a material where it is possible to switch between two very different phases in a way that involves strong piezoelectric, electric, and magnetoelectric effects [Diéguez and Íñiguez, Phys. Rev. Lett. 107, 057601 (2011)].

## P-9

### **Modification of NiO(111) surfaces by hydroxylation and carbonate formation**

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NiO is used as main or co-catalyst in heterogeneous catalysis. H<sub>2</sub>O, CO and CO<sub>2</sub> are commonly present at catalytic reactions and strongly interact with NiO surfaces. It is observed that they block surface sites or alter the surface structure by hydroxylation and carbonate formation and thereby poison the catalyst. In our study of the response of NiO to these gas phases we focused on the polar NiO(111) surface. The bulk-truncated structures are intrinsically unstable and especially susceptible to reactions with adsorbates. We performed spin-polarized GGA+U calculations for possible reconstructions of NiO(111) in contact with water, hydroxyl groups and protons or CO and CO<sub>2</sub>. A thermodynamic formalism was applied to deduce phase diagrams of the energetically most stable surface structures depending on temperature and pressure conditions.

The O-H phase diagram is dominated by a fully hydroxylated (1x1)-OH surface at ambient and low temperature UHV conditions and an adsorbate free (2x2)-O-octopolar structure after high temperature annealing. A transformation between these two stable phases includes not only the adsorption or desorption of water molecules but also the diffusion of Ni and O surface atoms. NEB calculations for reaction barriers of subprocesses of this phase transformation explain the experimentally observed high thermal stability of surface hydroxylation.

The interaction of CO and CO<sub>2</sub> with NiO(111) leads to the formation of tridentate carbonate complexes including O surface atoms which are interconnected by Ni surface atoms. Again, the molecules strongly alter the surface configuration. A transition path between adsorbate covered and adsorbate free surface structures has to involve a mass transport of Ni and O surface atoms. As expected from our theoretical results, a high thermal stability of carbonates is observed in experiment. We showed that the adsorption of small molecules on NiO(111) alters the surface considerably. These modifications have to be considered when modeling catalytic reactions.

## P-10

### Calculation of the Distribution of Current in MMX Polymers: the Case of $\text{Pt}_2\text{I}(\text{S}_2\text{C}_2\text{H}_3)_4$

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We present an *ab initio* study of the electronic band structure and probability currents of the quasi-one-dimensional (1D) MMX polymer  $[\text{Pt}_2(\text{CH}_3)_4\text{I}]_n$ , in the framework of density functional theory. Probability currents are calculated per atom by following the same concept used in Mulliken population analysis. We confirm the metallic band structure of the polymer reported in previous studies. Results of the current density calculations suggest the importance of both the Pt-Pt-I chain and the S atoms in the conductivity of the polymer.

## P-11

### Wurtzite-like Structures of Transition Metal Monoxides

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Transition metal monoxides (MnO, FeO, CoO, NiO) are well-known antiferromagnets that crystallize in the rock-salt lattice. They are used in a wide range of applications, from magnetic devices to catalysis, where often interface or surface properties perform a fundamental role. Their bulk structure has been largely studied as a model system to understand the description of exchange and correlation effects within a density-functional-theory (DFT) framework. Yet, there is controversy about their classification as Mott or charge-transfer insulators, the interplay between structure and magnetism, or even the phase diagram under different conditions.

Several bulk phases of CoO or FeO can be obtained preserving the hexagonal symmetry along the [111] direction [1]. Furthermore, particularly for CoO, recent evidence has been reported of the possibility to stabilize wurtzite nanostructures and surface terminations [2]. Under reduced dimensionality, the bulk phase diagram can be significantly altered, opening an intriguing field to manipulate the ionicity, magnetism and conductivity of these oxides.

Here we present our results about the stability of wurtzite-like terminations at the (111) surfaces of FeO and CoO, analyzing the implications in the electronic and magnetic properties. We employ first-principles calculations based on DFT, introducing corrections to the exchange-correlation term in order to reproduce the electronic gap at the bulk. We demonstrate that the results obtained for surfaces can be extended to low-dimensional structures, both unsupported slabs and ultrathin films grown on metal substrates. We will also discuss the effect of the exchange-correlation term in the phase diagram obtained.

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## P-12

### Beyond the Hubbard Model: a Realistic Description of Phase Transitions within the GW Approximation

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The central concept of the single-band Hubbard model is the competition for the electrons between the tendency to localize for the on-site effective Coulomb repulsion  $U$  and the opposite tendency to hybridize and spread over other lattice sites, which gives rise to a finite bandwidth  $W$ . By varying the  $U/W$  ratio it is possible to obtain a transition from localized to itinerant electronic states.

The realisation of this concept can be found in correlated electron materials, where by applying pressure it is possible to induce a transition between high-spin insulating and low-spin metallic phases.

Here we will discuss metal-insulator transitions in prototypical real systems (e.g. MnO or NiS<sub>2</sub>) using the parameter-free GW approximation of many-body perturbation theory [1]. We will show that the GW approximation is a very useful tool to understand the effects of electronic correlations across the phase transition.

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**P-13**

**First-principles Investigation of the Structural Phases and Enhanced Response Properties of the  $\text{BiFeO}_3$ – $\text{LaFeO}_3$  Multiferroic Solid Solution**

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We present a first-principles study of the BLFO solid solution formed by multiferroic  $\text{BiFeO}_3$  (BFO) and the paraelectric antiferromagnet  $\text{LaFeO}_3$  (LFO). We discuss the structural transformations that BLFO undergoes as a function of the La content  $x$ , and the connection of our results with the existing crystallographic studies. We find that, in a wide range of intermediate compositions, BLFO presents strongly competitive phases that are essentially degenerate in energy. Further, our results suggest that, within this unusual morphotropic region, an electric field might be used to induce a paraelectric-to-ferroelectric transition in the compound. We also discuss BLFO's response properties and show that they can be significantly enhanced by partial substitution of Bi/La atoms in the pure BFO and LFO materials. We analyze the atomistic mechanisms responsible for such improved properties, and show that the effects can be captured by simple phenomenological models that treat explicitly the composition  $x$  as a variable of a Landau-like potential.

**Momentum-space Finite-size Corrections for Quantum Monte Carlo Calculations**

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Extended solids are frequently simulated as finite systems with periodic boundary conditions, which due to the long-range nature of the Coulomb interaction may lead to slowly decaying finite-size errors. In the case of Quantum-Monte-Carlo simulations, which are based on real space, both real-space and momentum-space solutions to this problem exist. Here, we describe a hybrid method which using real-space data models the spherically averaged structure factor in momentum space. We show that (i) by integration our hybrid method exactly maps onto the real-space model periodic Coulomb interaction (MPC) method and (ii) therefore our method combines the best of both worlds (real-space and momentum-space). One can use known momentum-resolved behavior to improve convergence where MPC fails (e.g., at surface-like systems). In contrast to pure momentum-space methods, our method only deals with a simple single-valued function and, hence, better lends itself to interpolation with exact small-momentum data as no directional information is needed. By virtue of integration, the resulting finite-size corrections can be written as an addition to MPC.

## Band Structure of Bismuth Telluride: A Challenge for Theory and Experiment

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In the past, bulk bismuth telluride ( $\text{Bi}_2\text{Te}_3$ ) has been intensively investigated by both, experiment and theory, because of its outstanding thermoelectric properties. In particular doping with Sb or Se resulted in the highest thermoelectric figure of merit (ZT) values achieved so far. Several density functional theory (DFT) studies focused on the correct description of the valence band extrema (VBE) and conduction band extrema (CBE) [1]. This turned out to be a very challenging task for band structure calculations due to the strong spin orbit interactions (SOI) that is responsible for the small band gap of  $\text{Bi}_2\text{Te}_3$  ( $\sim 150$  meV) and the six-fold degeneracy of the VBE and CBE. It is believed that the latter is an important feature of the band structure that supports the extraordinary thermoelectric ZT value [2].

Recently  $\text{Bi}_2\text{Te}_3$  has again attracted much interest. Similar to graphene, atomically-thin crystalline films of  $\text{Bi}_2\text{Te}_3$  and  $\text{Bi}_2\text{Se}_3$  have been obtained by exfoliation [3]. In rapid succession,  $\text{Bi}_2\text{Te}_3$  and the related VA-VIA narrow gap semiconductors  $\text{Bi}_2\text{Se}_3$  and  $\text{Sb}_2\text{Te}_3$  have been identified as strong three dimensional (3D) nontrivial topological insulators (TIs) that exhibit topological behavior up to high temperatures and the simplest surface state possible: a single Dirac cone [4]. In these so-called *next generation* TIs, the strong SOI causes *band inversion*, i.e., the usual ordering of the valence band (mainly VIA-atom  $p$ -states) and conduction band (mainly VA-atom  $p$ -states) is inverted at the zone center ( $\Gamma$  point).

Motivated by the possible application of these materials in electronic and spintronic devices, many experimental and DFT investigations [5] have been reported within the last few years. Concerning the latter, recent studies again focus on the band structure of the materials, in particular on the SOI and the degeneracy of the VBE and CBE. However, the results of several DFT [1] as well as GW calculations [6] are still controversial regarding to (i) the energy difference of the two 6-fold VBEs, (ii) their positions in  $\mathbf{k}$ -space, and (iii) the degeneracy of the two CBEs. In the present work, we report on DFT calculations using hybrid functionals as implemented in the Vienna Ab initio Simulation Package (VASP). We show that a thorough crystal structure optimization and the inclusion of SOI for the tellurium atoms is important for an accurate description of the band structure of  $\text{Bi}_2\text{Te}_3$ . Furthermore, the exact exchange included by hybrid functionals counteracts the SOI and thus significantly changes the band gap as well as the CBE's position in  $\mathbf{k}$ -space and consequently its degeneracy.

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## P-16

### Spin-flip Hot Spot Structure in the Pb/Ge(111) Surface

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Heavy element surfaces have become an ideal testing ground for investigating the nature and effects of the relativistic spin-orbit interaction in low dimensional systems. In this work, we perform fully relativistic first principle calculations on optically induced spin-flip transitions between the metallic surface states of the Pb/Ge(111) surface. We calculate the spin-flip matrix elements following an approach based on the interpolation of maximally localized Wannier functions. The obtained results show a very high localization of the spin-flip transition probability in several hot spots in momentum space. We find that the origin of the hotspot structure is closely connected to the rapid variations of the momentum dependent surface spin-polarization. Furthermore, it is found that the location of the hot spots depends on the polarization of the applied electric field, allowing the manipulation of the spin-flip properties.

## P-17

### Role of Non-local Exchange in the Electronic Structure of Correlated Oxides

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Transition-metal oxides (TMO) with partially filled d or f shells are a prototype of correlated materials. They exhibit very interesting properties, like metal-insulator phase transitions (MIT) [1]. In this work we consider several TMO insulators in which Kohn-Sham LDA band structures are metallic: VO<sub>2</sub>, V<sub>2</sub>O<sub>3</sub>, Ti<sub>2</sub>O<sub>3</sub>, LaTiO<sub>3</sub> and YTiO<sub>3</sub>. In the past, this failure of LDA has been explained in terms of its inadequacy to capture the strong interactions taking place between correlated electrons. In the spirit of the Hubbard model, possible corrections to improve onsite correlation are the LDA+U [2] and LDA+DMFT [3] approaches. Here we make use of the HSE06 hybrid functional [4]. We show that, without invoking strong-correlation effects, the contribution of the non-local Fock exchange is essential to correct the LDA results, by curing its delocalization error. In fact, HSE06 provides insulating band structures and correctly describes the MIT in all the considered compounds [5]. We further discuss the advantages and the limitations of the HSE06 hybrid functional in correlated TMO.

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**P-18**

## **$O(N^3)$ Implementation of Hedin's GW Approximation**

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Hedin's GW approximation has been extensively applied in electronic structure calculations to determine HOMO and LUMO levels, line widths and total energies. Furthermore, our understanding of electronic transport benefits from the improved description of the one-electron Green's functions that is provided by Hedin's GW approximation. The screened Coulomb interaction that is a key ingredient of GW approximation is also necessary in the set up of the Bethe Salpeter equation for electron hole pair propagation. Present state of the art realizations of GW for non periodic systems are capable of treating relatively large molecules containing up to hundred atoms. However, the computational cost of GW calculations still remains prohibitive for many interesting applications in the emerging field of organic semiconductors. In this work, we would like to present our approach to Hedin's GW approximation. Our approach scales as  $O(N^3)$  with the number of atoms  $N$  and it provides the full frequency-dependent self-energy of the molecule. The key features of our approach are i) exploiting the locality of a certain basis in the set of orbital products, and ii) treating the frequency dependence of relevant quantities by means of their spectral functions. We will present the method along with several applications.

**P-19**

**Fully-atomistic First-principles Approach to the Temperature-dependent Lattice-dynamical Properties of Perovskite Oxides**

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We present a methodology for the parametrization of effective Hamiltonians for ferroelectric perovskites that provides a fully atomistic description of the materials. The parameters in our effective models are obtained from first-principles calculations; no experimental input is used. The potential energy surface is represented by a truncated Taylor expansion around the ideal cubic perovskite structure and is, up to second order, exactly equivalent to the first-principles computed one. Higher order terms are determined by fitting to the first-principles energetics and phonon dispersion relations of the relevant low-symmetry phases.

By treating all structural degrees of freedom explicitly our models allow us to investigate the competition between the soft modes that drive the ferroelectric phase transitions in these materials and other, secondary modes. Our method's ability to capture these interactions constitutes a considerable improvement upon earlier approaches.

We will show our newly parametrized effective Hamiltonian for the prototypical ferroelectric compound  $\text{PbTiO}_3$  and discuss its temperature dependent properties.



**P-20**

## **Disorder Effects in Si/Ge, Diamond -structured Semiconductors**

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We apply recent developments for the first-principles study of disordered systems to the particular case of Si-Ge semiconductors in a diamond (A4) structure.

Making use of beyond single-site developments of the coherent potential approximation, we consider the impact of short range ordering on properties of interest for practical device applications. The extent of disorder-to-order effects is investigated in its implications on equilibrium lattice parameter, electronic structure and band gap, together with different degrees of clustering, and other forms of interstitial defects. Results are also compared with alternative supercell-based approaches.

## P-21

### Tight binding model for C/BN interfaces

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The recent advances in graphene synthesis and growth control, has fostered research in other 2-dimensional systems. In particular, hexagonal boron nitride (h-BN) has emerged as a promising compound for patterning graphene and tune its electronic and mechanical properties at will. The compatibility between graphene and BN in their lattice parameters makes it possible the fabrication of hybrid systems with isolated regions of each compound [1]. DFT calculations have shown that for hybrid monolayers made of graphene nanoribbons (GNR) embedded in BN layers, the electronic behavior can be semiconductor, semimetal or half metal, depending on the ratio between GNR and BN widths [2]. The potential energy difference at the interface, the polarization of BN and the electronic screening in the GNR are the main factors that determine the characteristics of the band structure. In this work, we obtain tight-binding (TB) parameters from Siesta DFT calculations by means of maximally localized Wannier functions. Zigzag and armchair interfaces are considered for the parametrization. For zigzag, the on-site energies are found to be dependent on the distance from the edge, and on the nature of the edge (B- or N-terminated). With these values of TB parameters, a general model is proposed and applied in the study of different geometries of hybrid systems. The half-metallicity of zigzag interfaces is well represented as well as the band gap for armchair systems. Other systems studied are hexagonal quantum dots and layers composed of ribbons with variable width connected by zigzag interfaces.

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# Quantum Confinement Effect in the NH<sub>3</sub> Molecular Doping of Silicon Nanowires

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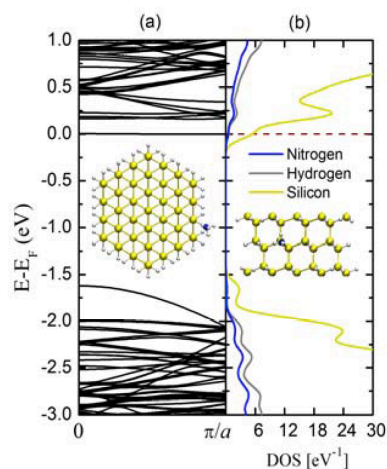
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We report *ab-initio* calculations on Silicon Nanowires (SiNWs) oriented along the [112], [110], [100] and [111] directions based on density functional theory (DFT). The influences of the molecular doping and quantum confinement on the electronic properties onto SiNWs are studied [1]. The possibility that an adsorbed molecule could provide shallow electronic states that could be thermally excited have received less attention than substitutional impurities and could potentially have a high impact in the doping of SiNWs. With such an approach one would simultaneously get rid of two problems that bedevils SiNW doping: (i) the competition between catalyzed and uncatalyzed incorporation of the impurities, often leading to sizeable disuniformities in the dopant concentration [2]; however, this *in-situ* approach does not always give favorable results [3], (ii) the need to carry out demanding annealing cycle to promote diffusion in *ex-situ* doping [4,5].

We present results for SiNWs with a diameter of 1.5 nm oriented along the [112], [110], [100] and [111] and the effect of quantum confinement on electronic properties for three different diameters of SiNWs in the [111] direction doped with NH<sub>3</sub>. The Fig. 1 (a) shows the band structure of SiNW doped with NH<sub>3</sub> in the [111] direction. It can be seen SiNW that the adsorbed molecule contributes with a localized state close to the conduction band edge, where it pins the Fermi level. Therefore the adsorbed molecule is found to be an efficient donor, as carriers can be thermally excited into the conduction band. More specifically we have found that NH<sub>3</sub> requires less energy to adhere to {110} faces, regardless of the growth orientation of the SiNWs. The molecular nature of these states are further supported by the projected electronic density of states, where projections are made on N, H and Si [Fig. 1(b)]. There it can be seen that the localized state is almost exclusively made up of N and H contribution, thus it is localized at the molecule adsorption site.

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**Figure 1.** SiNW doped with NH<sub>3</sub> in the [111] direction:

(a) Electronic band structures

(b) Projected electronic density of states

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**P-23**

## **Polyhedral Heteroborane Quantum Chemistry**

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Boron chemistry does not have the simplified detailed understanding of classical organic chemistry. However, the peculiar electronic structures admitted for boron species yields a rich variety of different interactions which emerge as a voyage between the worlds of organic, inorganic, and metal chemistry. Here, we report on reaction mechanisms and properties of monomeric, dimeric and other (hetero) borane clusters in their ground and excited electronic states, as a base for predicting the properties of complex polyhedral boron-based molecular architectures, especially based upon the icosahedral  $B_{12}H_{12}^{2-}$  moiety.

## P-24

### Linear-Scaling First-Principles Calculations of Point Defects in the MgO Ceramic

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We have used the order- $N$  functional minimization methods implemented in the SIESTA code to perform *ab initio* supercell computations of native point defects in bulk magnesium oxide. We investigate the energetics, structural and electronic properties of a vacancy and interstitial atom with different charge states, and of several atomic arrangements of neutral interstitial pairs and Schottky defects.

For the isolated defects, we find minimum formation energies corresponding to the full formal charge state, except for the O interstitial and vacancy cases showing charge transition levels (0/2-) and (2+/0) for values of the chemical potential of the electrons of 4 and 2.5 eV above the valence band maximum, respectively. The atomic structure of an extra O<sub>i</sub> atom strongly depends on its charge state  $q$ : for the nominal formal charge ( $q=2-$ ) the interstitial atom remains in the center of a cube of ions, whereas for a  $q=0$  state the extra atom forms a dumb-bell interstitial along the  $\langle 111 \rangle$  direction.

Defect pair arrangements of 1<sup>st</sup>-, 2<sup>nd</sup>- and 3<sup>rd</sup>-neighbor configurations for divacancies and up to 5<sup>th</sup> neighbor geometries for di-interstitials were evaluated. We obtain an overall lowest formation energy for the nearest neighbor configuration in both defect types. Interestingly, interstitial atoms in the 2<sup>nd</sup>- and 5<sup>th</sup>-neighbor configurations move towards lattice sites of same species during relaxation, displacing lattice atoms to otherwise form a 1<sup>st</sup>-neighbor di-interstitial defect in the supercell. Computationally, the  $O(N)$  approach yields accurate results ( $\sim 0.01$  eV/atom) even at relatively short localization radii (10 Bohr), which will make it the method of choice for studies of larger defect aggregates.

**P-25**

**Photoemission Spectra of Hydroxylated MgO(100) from *Ab Initio* Molecular Dynamics**

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*Ab initio* molecular dynamics has been used to investigate photoemission O1s core level shifts (CLS) of hydroxylated MgO(100). Rapid proton-exchange at elevated temperatures yields broad features in the simulated photoemission signal, which is in good agreement with recent experimental observations [1]. Moreover, the results provide further evidence that the stable structure of hydroxylated MgO(100) consists of a partly dissociated water monolayer. Analysis of the CLS for adsorbed hydroxyl groups at different coverage reveals a pronounced effect on hydrogen bonding to neighboring H<sub>2</sub>O molecules. The inclusion of exact exchange by the use of the hybrid PBE0 functional leads to quantitatively similar results as the gradient corrected PBE functional.

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## P-26

### Electronic Properties and Structure of 1d Ceria Materials: From Atomistic to Nanoscale Models

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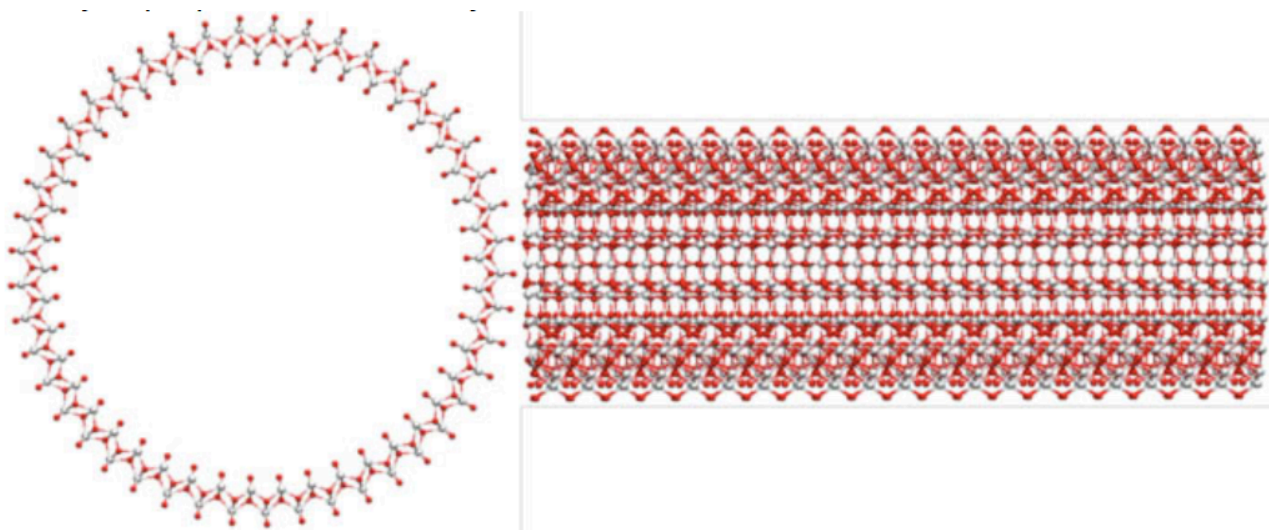
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Very recently, one dimensional ceria (1D), nanotubes (NT) and nanorods, have been reported as catalyst for the water gas shift (WGS) reaction at low temperature [1]. Theoretically it is important to stress that the electronic structure of reduced ceria materials constitutes a challenge in density functional theory (DFT) calculations due to the strongly correlated nature of the 4f electrons [2]. To the best of our knowledge there is no theoretical report on the electronic structure and properties of low dimensional ceria materials.

In this work we present a theoretical study by means of DFT calculations based on the B1WC functional of the geometry and electronic structure of single- and multi-layered ceria NT. Lattice parameters, strain energies, and density of states (DOS) have been examined in order to rationalize the structural and electronic properties of these low dimensional materials. Negative strain energies found in some series of NT allows to explain the experimentally observed formation of stable ceria NT [3]. The observed trends in strain energies and electronic structure (DOS) allows to understand the origin of the catalytic properties of these systems.



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**P-27**

**vdW-DFT Calculations in CH<sub>4</sub> and CO<sub>2</sub> Hydrates**

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We present ab initio results at the density functional theory level of methane and carbon dioxide hydrates, which include van der Waals interactions in a full ab initio treatment of the non-local correlation energy. It is found that van der Waals interactions dominate the energy, kinetics and stability of these inclusion compounds. The maximum absorption capacity and the maximum hydrocarbon size are calculated. A good description of the diffusion activation energies is also shown.



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Nanowires, and in particular silicon nanowires (SiNWs), are among the most exciting and promising building blocks for future nanoelectronics applications and have attracted the interest of many researchers around the world. Significant progresses have been achieved, especially in the latest decade, both from the experimental and the theoretical viewpoint.

Up to now, a significant overlap between the theoretical predictions and the experimental realizations

was still lacking, because nanowires that can be routinely grown to date have typical diameters ranging from 50 to 200 nm, while those that can be efficiently studied with electronic structure methods, reach 2-3 nm at most.

Nonetheless, these theoretical results are far to be regarded as bare academic exercises. On the contrary, the real interest of these studies is that they constitute an anticipation of most urgent problems that will have to be dealt within the next generation nanowires, when their characteristic sizes will really approach the quantum limit.

Here we review the recent progresses in the theoretical modeling of Si nanowires, the increasing overlap with experimental results and we discuss the future perspectives for a nanowires-based electronics, outlining the research agenda for nanowire-based devices to come [1].

We focus on nanowires with diameters below 10 nm, where quantum effects become important and the properties diverge significantly from those of bulk silicon. These wires can be efficiently treated within electronic structure simulation methods and will be among the most important functional blocks of future nanoelectronic devices. Firstly, we review the structural properties of silicon nanowires, emphasizing the close connection between the growth orientation, the cross-section and the bounding facets. Secondly, we discuss the electronic structure of pristine and doped nanowires, which hold the ultimate key for their applicability in novel electronic devices. Finally, we revise transport properties where some of the most important limitations in the performances of nanowire-based devices can lay. Many of the unique properties of these systems are at the same time defying challenges and opportunities for great technological advances.

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## P-29

### Theoretical Methods for the Calculation of the Dipole Moment of Functionalized Carbon Nanotubes

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We have investigated different methodologies based on first-principles calculations in order to obtain reliable values for the dipole moment of a functionalized carbon nanotube. Often, in the literature, this is calculated by considering a finite nanotube in which the dangling bonds at the edges are terminated by hydrogen atoms. Alternatively, a capped nanotube might be considered. However, these artificial terminations can lead to strong, spurious changes in the electronic structure of the nanotube. For instance, an inadequate termination may close the band gap of a semiconducting nanotube, due to the appearance of edge states. Thus, the calculated dipole moment of the resulting finite-size system ( $\int \mathbf{r} \rho(\mathbf{r}) d\mathbf{r}$ ) does not lead to the right results, due to charge sloshing between these edge states. In order to obtain reliable dipoles, we have considered functionalized carbon nanotubes terminated also by hydrogen atoms, but taking into account the Clar sextet rule. This rule states that the maximal generalized Clar structure contributes the most to the resonance energy. Thus, the Clar structure with maximum number of aromatic rings is expected to have an electronic structure close to an infinite nanotube. In addition, we have analyzed the convergence of the obtained dipole as a function of the length of the carbon nanotube and the distance between periodic copies for DFT programs working with periodic boundary conditions such as *SIESTA*. Finally, we compare these results with those obtained by the dipole moment using the Berry phase approach.

## P-30

### First-Principles study of interface structure and energy of Fe/NbC

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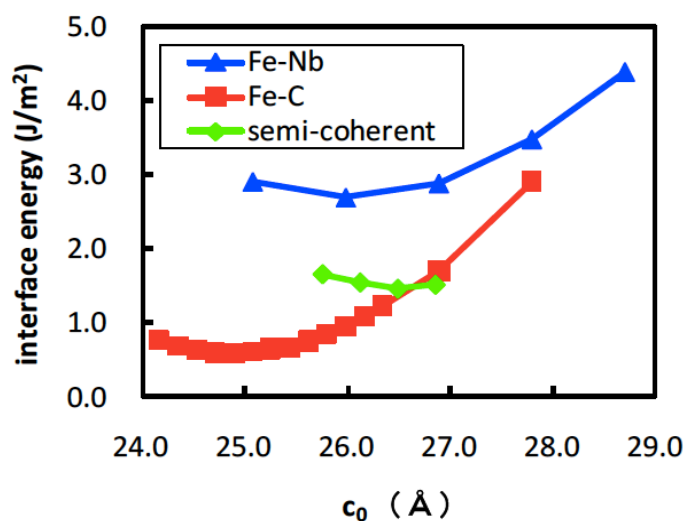
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The precipitates in steel play an important role to strengthen steel. One of the important factors of controlling growth of the precipitate is interface energy between precipitate and iron. The NaCl type precipitates are reported to have the Baker-Nutting orientation relationship with bcc iron, namely, (100)precipitate//[(100)iron and [010]precipitate//[011]iron. The interface between precipitate and iron changes from coherent to semi-coherent due to growth of the precipitates. Interface structure and energy were calculated for coherent interface and extended to semi-coherent interface within the Peierls-Nabarro framework in the previous literature [1]. The study omitted atomic relaxations except for the interphase separations, because it needs to treat more than one thousand atoms. In this study atomic relaxations are performed for all 1463 atoms in the unit cell by the use of  $O(N)$  method of large scale first-principles electronic structure calculation [2]. The interphase separation between Fe and NbC layers of the semi-coherent interface is close to that of the coherent interface where Fe atom is located next to Nb atom. The interface energy of the semi-coherent interface is the value between the coherent interface energy where Fe atom is located next to Nb atom and that where Fe atom is located next to C atom.

The numerical calculations were carried out on TSUBAME2.0 at Global Scientific Information and Computing Center of Tokyo Institute of Technology supported by the MEXT Open Advanced Research Facilities Initiative.

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## P-31

### Band gap control by tuning inversion degree in $\text{CdIn}_2\text{S}_4$ spinel

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$\text{CdIn}_2\text{S}_4$  spinel formula unit is  $(\text{Cd}_{1-x}\text{In}_x)[\text{In}_{2-x}\text{Cd}_x]\text{S}_4$  having in the perfectly direct spinel, Cd and In respectively in the tetrahedral and octahedral positions. The experimental value of inversion degree is around  $x=0.20$  then  $\text{CdIn}_2\text{S}_4$  is almost considered a direct spinel. Our work focuses on a thermodynamical analysis of the tetrahedral/octahedral cation inversion study inside  $\text{CdIn}_2\text{S}_4$  spinel. The Site Occupancy Disorder (SOD) program [1] had been a powerful tool to obtain the different inequivalent configurations of the disordered sites.

We demonstrate using the thermodynamical parameters that  $\text{CdIn}_2\text{S}_4$  have almost all their Cd/In in tetrahedral/octahedral cationic positions not exchanged and that the minimum of free energy correspond to an inversion which is coherent with the experimental value reported. The present findings are proposed as a novel theoretical methodology to obtain the exact degree of inversion in different spinels. Using the appropriate inversion degree the band-gap can be adjusted, which can be applied in the optimization of some photovoltaic processes.

Furthermore, phonon frequencies to determine vibrational total energy, and assignation of the active modes was also determined. The atomic configurational interaction using the configurational free energy contribution added to the vibrational free energy obtained gave us the complete theoretical approach to obtain the exact inversion degree. The change in temperature lead a change in the inversion degree which is related with the band-gap, then controlling temperature, the inversion degree can be tuned and we can also have a desirable value of band-gap of this promising photovoltaic material.

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## P-32

### First Principles Calculations of SnS<sub>2</sub> Layered Semiconductor Taking into Account the Van der Waals Interactions

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SnS<sub>2</sub> layered semiconductor doped with V was suggested as an intermediate band solar cell [1]. The different crystalline systems in which this layered material exist lead to different polytypes and this implies different characteristics. In this work we study the structural disposition of the most important polytypes of this layered material, the named 2h and 4h using the interatomic Van der Waals interactions that is present between the layers using two theories.

The Grimme [2] dispersion correction that is applied after each autoconsistent PBE electronic calculation, have intrinsically a semiempirical implementation which take into account the Van der Waals radius and the electrostatic interaction between the layers. The self-consistent Dion et al. [3] functional optimized for solids by Michaelides et al [4] on the other hand uses a complete theoretical approach.

In this work these two methods are applied to the layered SnS<sub>2</sub> polytypes and these two are compared and the results we will presented at this Conference, demonstrates the enhancement of the geometric parameters by the use of the Van der Waals interactions in agreement with the experimental values when either Grimme or the new functionals are used.

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## P-33

### Electronic Transport Between Platinum Contacts Through Graphene/Nanotubes Structures

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Recent studies have shown that highly conductive contacts are formed between platinum (Pt) contacts and carbon nanotubes (CNT)[1]. These contacts could be due to the formation of a graphene layer at the Pt-CNT interface[1].

We study electronic transport properties of CNTs with Pt contacts using first principles calculations. We have considered two situations: one where a layer of graphene had formed (and to where the CNT is covalently linked[2]) and the other where the CNT was in direct contact with the Pt surface. The simulations are performed within the density functional theory (DFT) and the Non-Equilibrium Green Function (NEGF) formalism. The calculations are performed with the SIESTA[3] code and its extension, TranSIESTA[4], for the electronic transport calculations, using strictly localised orbitals as basis sets.

After performing the relaxation in both systems, we found that the equilibrium distance between the graphene sheet and the Pt surface is of the order of 3.14 Å and the stable distance between the CNT and the Pt surface being of 2 Å. This fact brings us to the conclusion that the graphene sheet is decreasing the interaction of the CNT with the Pt contacts due to the larger distance between the Pt surface and the nanotube. As a consequence the overall transmission (when considering a wide range of energy) is higher in the second case (CNT directly on the Pt surface). We also perform transport calculations applying different voltages to the Pt contacts and we study the transmission eigenstates, the potential drop and the charge density drop.

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## P-34

### Study of the Effect of Disorder in Models of Topological Insulators by Means of the Lanczos Method

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Topological insulators (TIs) can be defined as non-trivial insulators possessing a gapped band structure in the bulk and gapless metallic edge/surface states due to the effect of the spin-orbit interaction (SOI) which are robust against disorder preserving time-reversal symmetry (TRS). In two dimensions (2D), SOI leads to the quantum spin Hall (QSH) phase showing gapless spinfiltered edge states. Recently, some works have addressed the effect of electron-electron interactions on these QSH insulators by combining the Kane-Mele Hamiltonian and the mean-field Hubbard model in a honeycomb lattice with zigzag edges giving rise to new and exotic electronic phases [1,2,3].

Here, we study the electronic properties of disordered diamond slabs containing more than 200000 atoms by means of the Lanczos method [4]. This method allows us to handle real size systems by tridiagonalizing a model Hamiltonian [5] which makes easier the computation of the density of states (DOS). The projection of such DOS onto the surface states makes possible to study the effect of different kind of bulk and surface disorder on the protected surface states of a topological insulator [6].

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**Germanium: Doped and Strained**

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Germanium (Ge) was used in fabricating the early electronic devices. Recent advances made in high  $k$ -dielectrics reengaged the interest in Ge. This interest stems from the higher electron and hole mobilities of Ge compared to Si in conjunction with the better thermal, and radiation hardness properties. The understanding of the defect processes and interactions is a prerequisite to optimize the properties Ge. Here density functional theory simulations are used to investigate the formation energies of  $n$ -type dopants (phosphorus, arsenic and antimony) paired with a vacancy in Ge for different charge states. Their activation energies of diffusion are also calculated and compared with the most recent experimental results, which show that the activation energy decreases as the size of the dopant atom increases. We also investigated the effect of strain on Ge and how this induces a change in the electronic structure. Both biaxial and uniaxial strains were applied along several important planes and directions were investigated. We found that Ge makes a transition from an indirect to direct band gap under biaxial (001) uniaxial [001], [110] and [111], with the latter providing the most efficient pathway for this transition.

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**P-36**

## **Molibdenum Atomic Wires Encapsulated in Carbon Nanotubes**

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Monoatomic chains of molybdenum encapsulated in single walled carbon nanotubes of different chiralities are investigated using density functional theory. We determine the optimal size of the carbon nanotube for encapsulating a single atomic wire, as well as the most stable atomic arrangement adopted by the wire. We also study the transport properties in the ballistic regime by computing the transmission coefficients and tracing them back to electronic conduction channels of the wire and the host. We predict that carbon nanotubes of appropriate radii encapsulating a Mo wire have metallic behavior, even if both the nanotube and the wire are insulators. Therefore, encapsulating Mo wires in CNT is a way to create conductive quasi one-dimensional hybrid nanostructures.

**P-37**

**Nuclear Quantum Effects on Dielectric and NMR Properties of Squaric Acid**

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Nuclear quantum effects, such as quantum delocalisation and tunneling, play an important role in many systems, in particular when hydrogen atoms and hydrogen bonding are present. The large isotope effect on the temperature of the ferroelectric phase transition in systems such as squaric acid ( $\text{H}_2\text{C}_4\text{O}_4$ ) and KDP ( $\text{KH}_2\text{PO}_4$ ) has been ascribed to quantum tunneling, but the nature of the nuclear quantum effects is intricate and still under debate. In this contribution I will present results from ab initio (DFT) path integral molecular dynamics (PIMD) simulations of squaric acid. In the past, evidence for the coexistence of order-disorder and displacive behaviour in this system has been obtained using high-resolution solid-state NMR experiments. We shed further light on these observations using theoretical calculations of NMR shielding constants in the gauge-including projector augmented wave (GIPAW) approach.

**Ab-initio Prediction of Giant Magnetoelectric Effects Driven by Structural Softness**

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Magnetoelectric (ME) multiferroics are materials in which electric and magnetic orders are coupled together [1], allowing for potential development of a variety of magnetic devices (e.g. memories, spin filters) whose behavior can in principle be controlled by application of an external voltage. Harvesting this property in the real-world applications is complicated by the scarcity of ferroelectrics which are magnetically ordered at room temperature [2] and the fact that they need to be good insulators and present sizable ME coupling at the same time. Because of the difficulties in experimental work on the materials, many key issues relating to their the physical properties remain to be addressed, which further hampers progress in this field.

We present a first-principles scheme for computing the lattice-mediated part of ME response of multiferroics [3] and show that it is possible to strongly enhance such a response by modifying elastic properties of these compounds [4]. Specifically, our calculations indicate that by inducing *structural softness*, the studied materials can be tuned toward giant ME effects. This observation does not depend on the material at hand; further, the structural softening can be achieved by a range of methods, from epitaxial growth to chemical substitution, which allows for a variety of experimental approaches depending on the specifics of the investigated compound.

We take the most promising ME multiferroic material to date: BiFeO<sub>3</sub> (BFO) [5], and present first-principles results for the calculated ME response tensor under a range of epitaxial strains which are demonstrably within reach of experiments [6]. We find that, as expected, the BFO under compressive epitaxial strain undergoes first order structural transition, which is accompanied by a narrow window of strain values in which it exhibits very large ME response at  $T=0$  K. This response in turn is expected to grow even higher as the temperature approaches the material's  $T_c$ . The calculated responses are further analyzed in a wide range of compressive strains in order to elucidate the underlying atomistic mechanism. It is found that the softness of AFD modes which connect the two competing phases is the main driving force for the ME response enhancement (in contrast to the Bi centered modes being the most active in the unstrained bulk BFO).

The presented results show a robust mechanism leading to large ME effects. Our simulations for BFO films show that the induction of structural softness results in effects comparable with the greatest ones ever measured for single-phase compounds. We hope our results will motivate the experimental exploration of this strategy either in BFO-based systems or in other compounds.

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**P-39**

## **Electronic structures and magnetic properties of LaFeAsO**

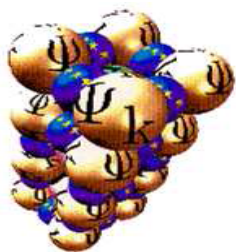
Changhyun Yi, Ju-Young Kim and Joo Yull Rhee\*

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Recently, high transition-temperature superconductivity was discovered in the iron-pnictide  $R\text{FeAsO}$  ( $R$ =rare-earths) family of materials. Among them,  $\text{LaFeAsO}$  undergoes a tetragonal to orthorhombic structural phase transition at  $\sim 160$  K followed closely by an antiferromagnetic ordering near 145 K. This material has also been reported to undergo a spin-density wave (SDW) transition near 150 K, based on specific heat, resistivity, and reflectivity measurements.

Through first-principles calculations we tried to understand the electronic structures and magnetic properties of  $\text{LaFeAsO}$ . We used full-potential linearized-augmented-plane-wave method in the antiferromagnetic ground state with orthorhombic phase. The physical origin of the SDW formation will be discussed.

# Psi-k Network : Towards Atomistic Materials Design



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## **PSI-K WORKSHOP FINANCE REPORT**

|                                 |   |
|---------------------------------|---|
| <b>Title of the Workshop</b>    | Computational Condensed Matter Physics, Materials Science and Nanoscience from First Principles |
| <b>Workshop Organisers</b>      | Pablo Ordejón, Jorge Iñiguez, Massimiliano Stengel, Daniel Sánchez-Portal                       |
| <b>Location of the Workshop</b> | Barcelona (Spain)   |
| <b>Dates of the Workshop</b>    | January 12-14, 2012   |
| <b>Total Grant from Psi-k</b>   | 5500  |

### **EXPENDITURE**

(Please complete the tables using numbers ONLY in the amounts fields - the spreadsheet will calculate the totals for you)

| <b>WORKSHOP DELEGATES / SPEAKERS</b>    |        |               |             |
|---|--------|---------------|-------------|
| Name and Country of Claimant            | Travel | Accommodation | Total (€'s) |
|   |        |               | € -         |
|   |        |               | € -         |
|   |        |               | € -         |
|   |        |               | € -         |
|   |        |               | € -         |
|   |        |               | € -         |
|   |        |               | € -         |
|   |        |               | € -         |
|   |        |               | € -         |
| <b>Total Travel &amp; Accommodation</b> |        |               | <b>€ -</b>  |

| <b>WORKSHOP REFRESHMENTS / CONFERENCE DINNERS</b> |              |                |                   |
|---|--------------|----------------|-------------------|
| Date  | Tea / Coffee | Lunch / Dinner | Total (€'s)       |
| 12/01/12  |              | € 3.187,20     | € 3.187,20        |
| 14/01/12  |              | € 2.695,00     | € 2.695,00        |
|   |              |                | € -               |
|   |              |                | € -               |
|   |              |                | € -               |
| <b>Total Refreshments</b>                         |              |                | <b>€ 5.882,20</b> |

| <b>MISCELLANEOUS EXPENDITURE</b> |             |
|----------------------------------|-------------|
| Details                          | Total (€'s) |
|                                  |             |
|                                  |             |
| <b>Total Miscellaneous</b>       | <b>€ -</b>  |

|   |                   |
|---|-------------------|
| <b>Total Travel &amp; Accommodation</b> | <b>€ -</b>        |
| <b>Total Refreshments</b>               | <b>€ 5.882,20</b> |
| <b>Total Miscellaneous</b>              | <b>€ -</b>        |
| <b>TOTAL EXPENDITURE</b>                | <b>€ 5.882,20</b> |

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