The Abdus Salam
International Centre
for Theoretical Physics

16th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods

10 - 12 January 2013

(Miramare, Trieste, Italy)

Co-sponsored by:
International School for Advanced Studies (SISSA)
CNR-IOM DEMOCRITOS Simulation Center
Psi-K Network
Asian Pacific Center for Theoretical Physics (APCTP)
Centre Européen de Calcul Atomique et Moléculaire (CECAM)
Consorzio per la Fisica - Trieste
Materials Computation Center (MCC)

Workshop Website:
http://cdsagenda5.ictp.it/full_display.php?ida=a12161

Organizing Committee:

Claudia FILIPPI University of Twente
The Netherlands
C. Filippi@utwente.nl

Richard M. MARTIN Stanford University, USA
rmartin@illinois.edu

Local Organizer:

Nadia BINGGELI ICTP, Trieste, Italy
binggeli@ictp.it

Scientific Committee:

W. Andreoni
(EPF Lausanne, Switzerland)
A. Baldereschi
(EPF Lausanne, Switzerland)
S. Baroni
(SISSA & DEMOCRITOS, Trieste, Italy)
C. Filippi
(University of Twente, The Netherlands)
G. Galli
(University of California at Davis, USA)
Xin-Gao Gong
(Fudan University, P.R. China)
J. Ihm
(Seoul National University, Korea)
E. Koch
(Forschungszentrum Jülich, Germany)
S. Louie
(University of California at Berkeley, USA)
R.M. Martin
(Stanford University, USA)
N. Marzari
(EPF Lausanne, Switzerland)
F. Mauri
(Université Pierre et Marie Curie, Paris, France)
S. Narasimhan
(JNCASR, Bangalore, India)
P. Ordejon
(ICMAB-CSIC, Barcelona, Spain)
L. Reining
(Ecole Polytechnique, Palaiseau, France)

C O N T E N T S

P R O G R A M M E

(as of 14 December 2012)

The Abdus Salam International Centre for Theoretical Physics

16th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods

Organizer(s): C. Filippi (The Netherlands), R.M. Martin (USA). ICTP Local Organizer: N. Binggeli
Trieste - Italy, 10 - 12 January 2013

Venue: Leonardo da Vinci Building Main Lecture Hall

Preliminary Programme

REGISTRATION AND WELCOME

10 January 2013

08:00 - 08:50 (Room: Leonardo da Vinci Building, Lobby)
--- REGISTRATION ---
All those attending the activity are required to complete registration formalities at the desk in the Leonardo Building entrance.

08:50 - 09:00 **Opening**

HIGH-THROUGHPUT AND FUNCTIONAL MATERIALS
Chairperson: Pablo Ordejón

10 January 2013

09:00 - 09:30 **Karsten Jacobsen** / *DTU, Denmark*
Atomic-scale design of energy materials

09:30 - 10:00 **Marco Bernasconi** / *University of Milano-Bicocca, Italy*
Simulation of phase change materials for data storage

10:00 - 10:30 --- Coffee Break ---

EXPLORING FUNCTIONAL MATERIALS
Chairperson: David Vanderbilt

10 January 2013

10:30 - 11:00 **Nicola Spaldin** / *ETHZ, Switzerland*
From transition metal oxides to cosmology with electronic structure calculations

11:00 - 11:30 **Raffaele Resta** / *University of Trieste, Italy*
Field-lattice coupling in flexoelectrics and magnetoelectrics

11:30 - 12:00 **Hong-jun Xiang** / *Fudan University, Shanghai, P.R. China*
General model for spin-order induced polarization in multiferroics

12:00 - 14:00 --- Lunch Break ---

AB-INITIO DYNAMICS
Chairperson: Sandro Scandolo

10 January 2013

14:00 - 14:30 **Ali Hassanali** / *ETHZ, Switzerland*
Water and its constituent ions under the microscope

14:30 - 15:00 **Bernd Ensing** / *University of Amsterdam, The Netherlands*
Recent progress in multiscale molecular dynamics simulation

15:00 - 15:30 **Jürg Hutter** / *University of Zurich, Switzerland*
Efficient implementation of Hartree-Fock exchange, MP2, and RPA for periodic systems within the GPW method

15:30 - 16:00 --- Coffee Break ---

QUANTUM DYNAMICS AND MOLECULAR SYSTEMS
Chairperson: Ralph Gebauer

10 January 2013

16:00 - 16:30 **Graham Worth** / *University of Birmingham, UK*
Treating non-adiabatic dynamics with the MCTDH method - from grid-based to direct dynamics

16:30 - 17:00 **Ivano Tavernelli** / *EPFL, Switzerland*
TDDFT-based non-adiabatic dynamics of complex molecular systems in external laser fields

17:00 - 17:30 **Thomas Miller** / *California Institute of Technology, USA*
Quantum Dynamics from Classical Trajectories: Direct simulation of charge transfer in enzymes and molecular catalysts

POSTER SESSION I
(Room:Adriatico Guest House (Lower Level 1))

10 January 2013

19:00 - 21:00 **Poster Session**
An informal buffet will be served to all participants during the poster session.

ELECTRONIC EXCITATIONS
Chairperson: Richard Martin

11 January 2013

09:00 - 09:30 **Steven Louie** / *University of California, Berkeley, USA*
Electronic excitations in solids and nanostructures: GW, GW-BSE, and beyond

09:30 - 10:00 **Lucia Reining** / *Ecole Polytechnique, Palaiseau, France*
A direct approach to the calculation of many-body Green's functions: beyond quasiparticles

10:00 - 10:30 --- Coffee Break ---

RPA AND BEYOND
Chairperson: Stefano Baroni

11 January 2013

10:30 - 11:00 **Patrick Rinke** / *Fritz Haber Institute, Germany*
Towards a unified description of ground and excited state properties: GW vs RPA and beyond

11:00 - 11:30 **Stefano de Gironcoli** / *SISSA, Italy*
RPA correlation potential in the adiabatic connection fluctuation-dissipation formalism

11:30 - 12:00 **Andrea Marini** / *ISM, CNR, Italy*
Competition between the electronic and phonon-mediated scattering channels in the out-of-equilibrium carrier dynamics of semiconductors: an ab-initio approach

12:00 - 14:00 --- Lunch Break ---

DMFT AND STRONGLY CORRELATED MATERIALS
Chairperson: Erik Koch

11 January 2013

14:00 - 14:30 **Michele Casula** / *Université Pierre et Marie Curie, France*
Dynamical screening effects from first principles: implications for low-energy models and application to the iron pnictides

14:30 - 15:00 **Eva Pavarini** / *Forschungszentrum Jülich, Germany*
Mechanism for orbital ordering in transition-metal oxides

15:00 - 15:30 **Ivan Leonov** / *University of Augsburg, Germany*
Total energy and force calculations for correlated materials

15:30 - 16:00 --- Coffee Break ---

QUANTUM MONTE CARLO
Chairperson: Sandro Sorella

11 January 2013

16:00 - 16:30 **George Booth** / *Princeton University, USA*
Towards a determinant space representation of the electronic wave function in the solid state

16:30 - 17:00 **Saverio Moroni** / *SISSA, Italy*
Minimum energy pathways from Quantum Monte Carlo

17:00 - 17:30 **Shiwei Zhang** / *College of William and Mary, USA*
Total energy calculations: an auxiliary-field many-body perspective

POSTER SESSION II (Room:Adriatico Guest House (Lower Level 1))

11 January 2013

19:00 - 21:00 **Poster Session**
An informal buffet will be served to all participants during the poster session.

SEARCH FOR NEW PHASES AND CLASSES OF MATERIALS (**Saturday**)
Chairperson: Emilio Artacho

12 January 2013

09:00 - 09:30 **Jeffrey M. McMahon** / *University of Illinois at Urbana-Champaign, USA*
Predicting the properties of ordinary matter under extreme conditions

09:30 - 10:00 **Joseph Bennett** / *Rutgers University, USA*
New classes of piezoelectrics, ferroelectrics, and antiferroelectrics by first-principles high-throughput materials design

10:00 - 10:30 --- Coffee Break ---

PROGRESS IN DEVELOPMENT OF NEW FUNCTIONALS (**Saturday**)
Chairperson: Michael Gillan

12 January 2013

10:30 - 11:00 **Andreas Görling** / *University of Erlangen-Nürnberg, Germany*
A new generation of density-functional methods based on the adiabatic-connection dissipation-fluctuation theorem

11:00 - 11:30 **Paola Gori Giorgi** / *Vrije Universiteit Amsterdam, The Netherlands*
Strong correlation in Kohn-Sham density-functional theory

11:30 - 12:00 **Julien Toulouse** / *Université Pierre et Marie Curie, France*
Combining wave-function and density-functional theories: range-separated hybrids, multiconfigurational hybrids, and double hybrids

12:00 - 12:30 **Andrea Ferretti** / *University of Modena, Italy*
Bridging density-functional and many-body perturbation theory: orbital-density dependence in electronic-structure functionals

12:30 - 12:45 **Closing remarks**

A B S T R A C T S

O F

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

(ordered according to the programme)

Atomic-scale design of energy materials

Ivano E. Castelli, Kristian S. Thygesen, Karsten W. Jacobsen

Center for Atomic-scale Materials Design, DTU Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark.

The design of new materials for more efficient production and use of sustainable and clean energy is of utmost importance for the standard of living all over the World the coming years. Efficient utilization of solar energy can take many forms including transforming the energy of the light into heat, electrical energy, or fuels.

In the talk I shall describe some computational efforts to design new materials related to solar energy in particular to the conversion of light into hydrogen fuel through water splitting. We have employed computational screening to search for stable semiconductor materials with an appropriate bandgap, band edge alignment, and with sufficient stability in an aqueous environment to be relevant for light-induced water splitting. In particular we have focused on a large amount of oxides, oxynitrides, oxysulfides, oxyfluorides, and oxyfluoronitrides in the cubic perovskite structure but also more generally materials in the ICSD database. The screening of bandgaps is performed using the so-called GLLB-functional which is shown to give reasonable estimates of bandgaps and light absorption for a number of different systems. The stability of the materials towards dissolution in water is investigated through the construction of Pourbaix diagrams combining DFT calculations and experimental information about solution energies.

The talk will also cover some recent efforts in using machine-learning techniques to develop new electronic density functionals. The functional construction uses Tikhonov regularization to obtain smooth functionals and employs bootstrapping to avoid overfitting. The new functionals are named Bayesian Error Estimation Functionals (BEEF) because they automatically offer error estimation on calculated results.

Simulation of phase change materials for data storage

G. C. Sosso[1], G. Miceli[1], S. Caravati[2], J. Behler[3], M. Bernasconi[1]

1. Department of Materials Science, University of Milano-Bicocca, Milano, Italy
2. Department of Chemistry and Applied Biosciences, ETH Zurich and USI Lugano, Switzerland
3. Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, Bochum, Germany

Chalcogenide phase change alloys ($Ge_2Sb_2Te_5$, GeTe and related materials) are the subject of extensive experimental and theoretical research because of their use in optical (DVD) and electronic (phase change memories, PCM) storage devices [1]. Both applications rely on the fast and reversible transformation between the crystalline and amorphous phases induced by heating either via laser irradiation (DVD) or Joule effect (PCM). The two states of the memory can be discriminated thanks to the large difference in optical reflectivity and electronic conductivity of the two phases.

In the last few years, molecular dynamics (MD) simulations based on density functional theory (DFT) have provided useful insights on the properties of phase change materials (see Ref. [1] for a review and Ref. [2] for some of our contributions). However, several key issues such as the crystallization dynamics and the thermal conductivity at the nanoscale, just to name a few, are presently beyond the reach of fully DFT simulations. A route to overcome the limitations in system size and time scale of DFT-MD is the development of classical interatomic potentials. Traditional approaches based on the fitting of simple functional forms are very challenging due to the complexity and variability of the chemical bonding in the crystal and amorphous phases revealed by DFT simulations. A possible solution has been demonstrated recently by Behler and Parrinello [3] who developed empirical interatomic potentials with close to DFT accuracy for several elemental systems by fitting a large DFT database with a Neural Network (NN) scheme. By means of this technique, we have recently developed an interatomic potential for GeTe [4] which is one of the compounds under scrutiny for applications in PCM.

After a brief review of our main DFT results on the properties of amorphous $Ge_2Sb_2Te_5$ and related materials, we will discuss large scale NN simulations (4000 atoms for 10 ns) of GeTe addressing several properties such as the fragility of the supercooled liquid close to the glass transition temperature [4] and the crystallization dynamics of the amorphous phase.

[1] D. Lencer, M. Salinga, and M. Wuttig, Adv. Mat. 23, 2030 (2011); M. Wuttig and N. Yamada, Nature Mater. 6, 824 (2007).
[2] S. Caravati *et al.*, Appl. Phys. Lett. 91, 171906 (2007); Mazzarello *et al.*, Phys. Rev. Lett. 104, 085503 (2010); G. C. Sosso *et al.*, Phys. Rev. B 83, 134201 (2011).
[3] J. Behler and M.Parrinello, Phys. Rev. Lett. 14, 146401 (2007)
[4] G. C. Sosso *et al.*, Phys. Rev. B 85, 174103 (2012); G. C. Sosso *et al.*, Phys. Rev. B 86, 104301 (2012); Physica Status Solidi B 249, 1880 (2012).

From transition metal oxides to cosmology with electronic structure calculations.

Nicola A. Spaldin

Materials Theory, ETH Zürich

What happened in the early universe just after the Big Bang? This is one of the most intriguing basic questions in all of science, and is difficult to answer because of insurmountable issues associated with replaying the Big Bang in the laboratory. One route to the answer is to use condensed matter systems to test the so-called "Kibble-Zurek" scaling laws for the formation of defects such as cosmic strings that are proposed to have formed in the early universe. In this talk I will show that a popular multiferroic material – with its coexisting magnetic, ferroelectric and structural phase transitions – generates the crystallographic equivalent of cosmic strings. I will describe how we used electronic structure calculations within the density functional theory framework to identify and quantify the behavior, and show experimental results of the first unambiguous demonstration of Kibble-Zurek scaling.

Field-Lattice Coupling in Flexoelectrics and Magnetoelectrics

Raffaele Resta

1. Dipartimento di Fisica, Università di Trieste, Italy.
2. DEMOCRITOS National Simulation Center, IOM-CNR, Trieste.

In piezoelectric crystals a uniform strain induces macroscopic polarization. Instead flexoelectricity is polarization induced by strain *gradient*; it is symmetry allowed even in high-symmetry crystals. The basic issue whether they are bulk properties has been settled in the 1970s for piezoelectricity, and is unsettled to this day for flexoelectricity. A first step towards a bulk theory of flexoelectricity has been achieved in Ref. [1], where only the simplest class of dielectrics was addressed: elemental cubic crystals. Subsequent work addressing more useful classes of crystals has stumbled over a major problem; possibly flexoelectricity needs a bold paradigm change.

In ordinary dielectrics the field $\mathbf{E}$ is coupled to the electronic polarization as well as to the lattice, via the ionic charges. This has three important consequences: (1) the static dielectric constant (or tensor) ε_0 is different form the electronic one ε_∞ (also called "clamped nuclei" dielectric constant); (2) the phonon spectrum is nonanalytic at short wavevector; (3) The zone-center phonon frequencies are related to the dielectric constants by the Lyddane-Sachs-Teller (1941) relationship, nowadays in every solid-state-physics textbook. In magnetoelectrics an electric field induces macroscopic magnetization, and a magnetic field induces electrical polarization. Both fields $\mathbf{E}$ and $\mathbf{H}$ contribute to the coupling on equal footing, and therefore the points (1−3) above need a complete reformulation; this has been recently achieved [2,3].

Two more specialized topics are possibly discussed. (i) To a first-principle theorist, the macroscopic fields of choice are $\mathbf{E}$ and $\mathbf{B}$, not $\mathbf{H}$: they enter e.g. the Kohn-Sham Hamiltonian. The solution of the $\mathbf{H}$ vs. $\mathbf{B}$ issue is provided. (ii) A magnetic field does not exert any force on a nucleus at rest: so which is the origin of the magnetic lattice coupling? The answer to this question is provided [3].

[1] R. Resta, Phys. Rev. Lett. **105**, 127601 (2010).
[2] R. Resta, Phys. Rev. Lett. **106**, 047202 (2011).
[3] R. Resta, Phys. Rev. B **84**, 214428 (2011).

General model for spin order induced polarization in multiferroics

Hongjun Xiang[1], *X.Z. Lu*[1], *J. H. Yang*[1], *X. G. Gong*[1], *M.-H. Whangbo*[2]

1. Key Laboratory of Computational Physical Sciences (Ministry of Education), State Key Laboratory of Surface Physics, and Department of Physics, Fudan University, Shanghai 200433, People's Republic of China
2. Department of Chemistry, North Carolina State University, Raleigh, North Carolina 27695-8204, USA

In recent years, we have theoretically studied the microscopic origin of ferroelectricity in different multiferroic systems. We proposed a general model [1-3] for spin-order induced ferroelectric polarization, which not only unifies the existing models for magnetic multiferroics, but also generalizes the spin-current induced polarization model. Based on the first-principles calculations, we explained the ferroelectricity induced by the proper-screw spin spiral [1], unraveled a novel magnetoelectric coupling mechanism in which the magnitude of the polarization is governed by the exchange striction with the direction by the spin chirality [2], proposed that the ferroelectricity in the chiral-lattice magnet Cu_2OSeO_3 is due to the unusual single-spin site term [3]. In addition, we also proposed an efficient approach to compute the first order derivatives of spin interaction parameters [4].

[1]. H. J. Xiang, E. J. Kan, Y. Zhang, M.-H. Whangbo, and X. G. Gong, "General Theory for the Ferroelectric Polarization Induced by Spin-Spiral Order", Phys. Rev. Lett. **107**, 157202 (2011).

[2]. X. Z. Lu, M.-H. Whangbo, Shuai Dong, X. G. Gong, and H. J. Xiang, "Giant Ferroelectric Polarization of $CaMn_7O_{12}$ Induced by a Combined Effect of Dzyaloshinskii-Moriya Interaction and Exchange Striction", Phys. Rev. Lett. **108**, 187204 (2012).

[3]. J. H. Yang, Z. L. Li, X. Z. Lu, M.-H. Whangbo, Su-Huai Wei, X. G. Gong, and H. J. Xiang, "Strong Dzyaloshinskii-Moriya Interaction and Origin of Ferroelectricity in Cu_2OSeO_3", Phys. Rev. Lett. **109**, 107203 (2012).

[4]. H. J. Xiang, E. J. Kan, Su-Huai Wei, M.-H. Whangbo, and X. G. Gong, "Predicting the spin-lattice order of frustrated systems from first principles", Phys. Rev. B **84**, 224429 (2011).

Water and its Constituent Ions Under the Microscope

Ali Hassanali[1], *Federico Giberti*[1], *Michele Parrinello*[1]

1. ETH-Z and University of Lugano

Here we use extensive *ab initio* molecular dynamics (AIMD) simulations to probe the complex hydrogen bond network of liquid water and its constituent ions, the proton and hydroxide. By inserting the directionality of the network in ring-like structures originally observed by Rahman and Stillinger, we unveil some "ground rules" in the cooperative organization of the water network. Directed rings are populated by water molecules acting as double-donors (DD), double-acceptors (AA) or single donor-acceptors (DA) in a ring. The closed directed topology requires that DD and AA waters always come in pairs resulting in directional correlations along the rings. The hydronium and hydroxide ions peturb the network via a collective effect on the distribution of the directed rings which results in "proton-wires" decorating both ions. The presence of these wires results in a broader distribution of pathways and timescales of proton and hydroxide transfer in water compared to the currently accepted picture of the Grottuss mechanism. The diffusion of both the proton and hydroxide goes through periods of burst in activity involving hops over several waters followed by resting periods. Long-range diffusion requires that the proton translocates from one ring to another. The solvent reorganization driving this activity is a multiscale and multidynamical process involving the coupling of the collective compressions of wires, water network restructuring and for the case of the excess proton, its umbrella-inversion motion.

Recent progress in multiscale molecular dynamics simulation

Bernd Ensing

University of Amsterdam, Science Park 904, 1098 XH Amsterdam, The Netherlands

Multiscale modeling techniques allow to simulate larger systems and longer time scales by reducing the level of detail in the model where and when possible. In this talk I will present two multiscale methods that we have recently developed.

The first method is path-metadynamics, which allows us to sample activated processes, such as chemical reactions, that take place on a time scale that is much longer than the accessible time of a straightforward molecular dynamics simulation. Path-metadynamics determines the most-likely reaction path as a function of (many) selected coordinates and obtains the free energy profile along this reaction path. As an example, I will show its application to unravel the light-activated conformational transition in photoactive yellow protein.

The second method is adaptive multiscale molecular dynamics, which we developed to study the interesting parts of a molecular system in atomistic detail, while including the environment with a reduced, coarse-grain, model. The boundaries of the atomistic/coarsegrain regions are open and the molecules that diffuse over adapt their resolution on the fly. I will briefly discuss the statistical mechanical consequences of such hybrid multiscale modeling and show its application to model the swelling of a polymer.

Efficient Implementation of Hartree-Fock Exchange, MP2, and RPA for Periodic Systems within the GPW Method

Jürg Hutter

Physical-Chemistry Institute, University Of Zurich, Switzerland

There is a strong increase in interest in wavefunction based electronic structure methods in recent years for condensed matter systems. Hybrid functionals and post Hartree–Fock methods, e.g. MP2 or random phase approximations have been investigated and it has been found that a considerable improvement over standard GGA density functionals can be achieved for selected properties and systems. Although these methods and their corresponding algorithms have been well studied in quantum chemistry over many years, new computational problems arise in condensed phase systems. Many of these problems are related to periodic boundary conditions and the use of special basis sets. The Gaussian and Plane Waves (GPW) method has been developed in order to combine the advantages of localized (chemistry aware) basis sets and the use of regular grids and plane waves for the description of electrostatic interactions in periodic systems. We will show that these combined advantages also hold, at least in part, for wavefunction based methods. We will present a family of algorithms that allow for an efficient calculation of Hartree–Fock exchange and post-HF energy terms. Accuracy and efficiency of these algorithms for hybrid density functional calculations will be documented. Finally, we will investigate the current limits for system size and structure sampling using post-HF methods.

Treating Non-adiabatic dynamics with the MCTDH method - from grid-based to direct dynamics

Graham Worth[1],

1. School of Chemistry, University of Birmingham, Edgbaston, B15 2TT, UK

The direct numerical solution of the time-dependent Schrödinger equation has become an essential tool for the theoretical study of fundamental molecular processes. The Multi-configuration time-dependent Hartree (MCTDH) method [1, 2] provides a powerful quantum dynamics algorithm, which enables us to include more degrees of freedom than other methods. This is particularly useful in the study of photochemistry, where non-adiabatic effects can couple the motion of a number of degrees of freedom leading to the need to simulate a multi-dimensional problem [3]. A benchmark example was a study of the pyrazine molecule including explicitely all 24 vibrational modes [4]. In a more recent example, simulations on benzene, combined with experiments made by the Fielding group at UCL, have uncovered a channel with ultrafast inter-system crossing that plays a role in the classic channel 3 problem [5].
MCTDH is, however, a grid-based method. And like all grid-based quantum dynamics methods is still restricted to small moelcules. To extend the method to larger and more general systems, we are developing a direct dynamics version, in which the potential surfaces are calculated on-the-fly using quantum chemistry calculations only when required by the system. The DD-vMCG method is fully quantum mechanical, and promises to have good convergence properties, which are essential for these expensive calculations [6].

References

[1] H.-D. Meyer, U. Manthe and L. S. Cederbaum, Chem. Phys. Lett. 165 (1990) 73.

[2] M. H. Beck, A. Jäckle, G. A. Worth and H.-D. Meyer, Phys. Rep. 324 (2000) 1.

[3] G. A. Worth, H.-D. Meyer, H. Köppel, L. S. Cederbaum and I. Burghardt, Int. Rev. Phys. Chem. 27 (2008) 569.

[4] A. Raab, G. Worth, H.-D. Meyer and L. S. Cederbaum, J. Chem. Phys. 110 (1999) 936.

[5] R. S. Minns, D. S. N. Parker, T. J. Penfold, G. A. Worth and H. H. Fielding, PCCP 12 (2010) 15607.

[6] G. A. Worth, M. A. Robb and B. Lasorne, Mol. Phys. 106 (2008) 2077.

TDDFT-based nonadiabatic dynamics of complex molecular systems in external laser fields

Basile F. E. Curchod[1], *Ursula Roethlisberger*[1], *Ivano Tavernelli*[1,2]

[1] Laboratory of Computational Chemistry and Biochemistry, Ecole Polytechnique Fédérale de Lausanne, Lausanne, 1015, Switzerland.

[2] ivano.tavernelli@epfl.ch

In the mixed quantum-classical description of molecular systems, only the quantum character of the electronic degrees of freedom is considered while the nuclear motion is treated at a classical level. In the adiabatic case, this picture corresponds to the Born-Oppenheimer limit where the nuclei move as point charges on the potential energy surface (PES) associated with a given electronic state. Despite the success of this approximation, many physical and chemical processes do not fall into the regime where nuclei and electrons can be considered decoupled. In particular, most photoreactions pass through regions of the PES in which electron-nuclear quantum interference effects are sizeable and often crucial for a correct description of the phenomena.

Recently, we have developed a trajectory-based nonadiabatic molecular dynamics scheme that describes the nuclear wavepacket as an ensemble of particles following classical trajectories on PESs derived from time-dependent density functional theory (TDDFT) [1]. The method is based on Tully's fewest switches trajectories surface hopping (TSH) where the nonadiabatic coupling elements between the different potential energy surfaces are computed on-the-fly as functionals of the ground state electron density or, equivalently, of the corresponding Kohn-Sham orbitals [2]. Alternatively, we can also capture nuclear quantum effects using Bohmian trajectories derived from quantum hydrodynamics [3].

Here, we present the theoretical fundamentals of our approach together with an extension that allows for the direct coupling of the dynamics to an external electromagnetic field [4] as well as to the external potential generated by the environment (solvent effects) [5]. The method is applied to the study of the photodissociation dynamics of simple molecules in gas phase and to the description of the fast excited state dynamics of molecules in solution.

[1] Tapavicza E., Tavernelli I., Rothlisberger U., Phys. Rev. Lett., 98 , (2007) 023001.
[2] Tavernelli I.; Tapavicza E.; Rothlisberger U., J. Chem. Phys ., 130, (2009) 124107 .
Tavernelli I., Curchod B.F.E., Rothlisberger U., J. Chem. Phys ., 131 , (2009) 196101.
Tavernelli I., Curchod B.F.E., Laktionov A., Rothlisberger U., J. Chem. Phys. , 133 , (2010) 194104.
[3] Curchod B.F.E., Tavernelli I., Rothlisberger U, Phys. Chem. Chem. Phys., 13, (2011) 3231.
[4] Tavernelli I., Curchod B.F.E., Rothlisberger U., Phys . Rev. A , 81 , (2010) 052508.
[5] Tavernelli I., Curchod B.F.E., Rothlisberger U., Chem. Phys, 391 , (2011) 101.

Quantum Dynamics from Classical Trajectories: Direct simulation of charge transfer in enzymes and molecular catalysts

Thomas F. Miller, III
Division of Chemistry and Chemical Engineering,
California Institute of Technology

Condensed-phase charge-transfer reactions are a central feature of many biological and synthetic catalytic pathways. The development of accurate, scalable methods to simulate and understand these reactions is thus a central challenge for chemical theory. In this talk, we will describe recently developed path-integral methods for the direct simulation of condensed-phase electron transfer, proton transfer, and proton-coupled electron transfer (PCET) reactions. Specific applications will include *(i)* characterization of the role of nanometer-scale protein fluctuations in facilitating enzyme-catalyzed hydrogen transfer and *(ii)* comparison of concerted vs. sequential reaction pathways for PCET in mixed-valence iron bi-imidazoline systems.

Electronic excitations in solids and nanostructures: GW, GW-BSE, and beyond

Steven G. Louie[1]

1. Department of Physics, University of California at Berkeley, and Materials Sciences Division, Lawrence Berkeley National Laboratory

In this talk, we discuss some recent progress in the use of the GW approach and its extensions to electronic excitations and related spectroscopic properties of materials and nanostructures. Inclusion of electron-hole interactions allows further *ab initio* study of optical properties. Several topics are discussed. We present results on excitonic effects in the optical spectra of graphene, in the form of a strong resonant exciton, and show how the prominent exciton features are altered by carrier doping and quasiparticle lifetime. We describe how calculations of electronic multiplet splittings are possible within the GW approximation. Finally, we show that the *ab initio* GW approximation overestimates the quasiparticle-satellite separation significantly in photoemission spectra and falsely predicts a plasmaron excitation. By including significant vertex corrections via the *ab initio* GW+cumulant approach, we demonstrate that the plasmon satellites may be accurately computed, explaining recent angle-resolved photoemission measurements, e.g., on graphene. Comparisons with experiments for all three cases are presented.

A direct approach to the calculation of many-body Green' s functions: beyond quasiparticles

Lucia Reining[1,2]

1. Laboratoire des Solides Irradiés, Ecole Polytechnique, 91128 Palaiseau, France
2. European Theoretical Spectroscopy Facility (ETSF)

Green's functions based methods are powerful tools to describe many properties of materials. For example, Hedin's GW approximation in the framework of many-body perturbation theory has become a standard approach for the calculation of the bandstructure of materials. However, the excitation spectra of interacting systems contains more than just quasiparticle peaks. Photoemission, for example, shows satellite structure that cannot be interpreted in a pure bandstructure picture. Perturbative approaches like GW often have difficulties to describe quantitatively, or even qualitatively, such correlation effects.

We are exploring a non-perturbative route to the calculation of interacting electron Green's functions. It is based on a set of functional differential equations relating the one-particle Green's function to its functional derivative with respect to an external perturbing potential [1]. We will discuss insight that one can gain from solving the equations for model systems [2], advances in the description of photoemission and absorption obtained by an approximate solution of the equations for real systems [3], and recent progress towards more and more complete solutions.

[1] L.P. Kadanoff and G. Baym, *Quantum Statistical Mechanics* (New York: Benjamin, 1962)
[2] G. Lani, P. Romaniello, and L. Reining, New J. Phys. **14**, 013056 (2012)
[3] M. Guzzo et al., Phys. Rev. Lett. **107**, 166401 (2011)

Towards a unified description of ground and excited state properties: *GW vs* RPA and beyond

Patrick Rinke

Fritz-Haber-Institut der Max-Planck-Gesellschaft
Faradayweg 4–6, 14195 Berlin

In the quest for finding an "optimal" first principles electronic structure method, that combines accuracy and tractability with transferability across different chemical environments and dimensionalities (e.g. molecules, wires/tubes, surfaces, solids), the treatment of exchange and correlation in terms of "exact-exchange plus correlation in the random-phase approximation (EX+cRPA)" offers a promising avenue. Likewise one can express the same level of theory in the Green's function context through the *GW* approximation, which has the additional advantage that quasiparticle spectra as measured by direct and inverse photoemission become accessible. In this talk I will contrast both approaches and present the latest results from our continuous assessment. We find that self-consistent (sc) *GW* provides excellent charge densities, which is particularly important for charge transfer systems [1]. Spectral properties for closed shell molecules are generally in good agreement with photoemission spectra, although a judicial choice of the starting point in perturbative G_0W_0 calculations can outperform scGW [1,2]. Other ground state properties do not improve over EX+cRPA calculations [1]. EX+cRPA, on the other hand, provides a good description of the ground state [3] even for challenging cases like chemical reaction barrier heights [4] and the f-electron metal Cerium [5]. The notorious underbinding of EX+cRPA can be corrected by going beyond RPA to renormalised second order perturbation theory (rPT2) [3] that gives the overall most balanced performance.

[1] F. Caruso, P. Rinke, X. Ren, M. Scheffler, and A. Rubio, Phys. Rev. B **86**, 081102(R) (2012)
[2] N. Marom *et al.*, arXiv:1211.0416
[3] X. Ren, P. Rinke, C. Joas, and M. Scheffler, J. Mat. Sci. **47**, 7447 (2012)
[4] J. Paier, X. Ren, P. Rinke, G. E. Scuseria, A. Grüneis, G. Kresse, and M. Scheffler, New J. Phys. **14**, 043002 (2012)
[5] M. Casadei, X. Ren, P. Rinke, A. Rubio, and M. Scheffler, Phys. Rev. Lett. **109**, 14642 (2012)

RPA Correlation Potential in the Adiabatic Connection Fluctuation-Dissipation formalism

Stefano de Gironcoli

Scuola Internazionale Superiore di Studi Avanzati (SISSA), via Bonomea 265, I-34136 Trieste, Italy

Calculations of correlation energies within the formally exact Adiabatic Connection Fluctuation-Dissipation (ACFD) formalism, within the Random Phase Approximation (RPA) for the exchange-correlation kernel, have been recently carried out for a number of isolated and condensed systems. The efficiency of such calculations has been greatly improved by exploiting iterative algorithms to diagonalize RPA dielectric matrices [1]. However for several systems correlation energies may significantly depend about the choice of input single particle wavefunctions [2]. We derive an expression for the RPA self-consistent potential based on Density Functional Perturbation theory and we present self-consistent RPA calculations for weakly bound molecular dimers, including the controversial case of Beryllium dimer. In this case the self-consistent determination of RPA potential is crucial to determine the stability of the system which however results to be unstable toward dissociation in separated fragments.

[1] H.-V. Nguyen and S. de Gironcoli, Phys. Rev. B 79, 205114 (2009); H. F. Wilson, F. Gygi, and G. Galli, Phys. Rev. B 78, 113303 (2008).

[2] Huy-Viet Nguyen and G.Galli, J. Chem.Phys. 132, 044109 (2010).

Competition between the electronic and phonon–mediated scattering channels in the out–of–equilibrium carrier dynamics of semiconductors: an *ab–initio* approach

Andrea Marini,

Istituto di Struttura della Materia of the National Research Council, Via Salaria Km 29.3, I-00016 Monterotondo Stazione, Italy.

Ultra–fast optical spectroscopy is a powerful tool for the observation of dynamical processes in several kind of materials. The basic time–resolved optical experiment is the so-called pump-probe: a first light pulse, the pump, resonantly triggers a photo-induced process. The subsequent system evolution can be monitored, for example, by the time–dependent transmission changes of a delayed probe pulse. The pump pulse photon energy, spectral width and peak intensity creates a certain density of electron-hole pairs in a more or less localized region of space. After the creation of the initial carrier density the time evolution of the single–particle and many–particle excitations is now governed by a non-trivial interplay between electron–electron scatterings and energy relaxation. De-phasing will be driven by different phenomena. One of the most important is the energy transfer to the atomic motion in form of phonon excitations.
In this talk I will present a novel approach based on the merging of Non-Equilibrium Green's function theory and Density Functional Theory to investigate the carrier dynamics following a pump excitation.
The case of bulk Silicon, a paradigmatic indirect gap semiconductor, is studied by using the Baym–Kadanoff equations. Both the electron–electron (e–e) and electron–phonon (e–p) self–energies are calculated fully *Ab–Initio* by using a semi–static GW approximation in the e–e case and a Fan self–energy in the e–p case. By using the generalized Baym–Kadanoff ansatz the two–time evolution is replaced by the only dynamics on the macroscopic time axis. The enormous numerical difficulties connected with a real–time simulation of realistic systems is overcomed by using a completed collision approximation that further simplifies the memory effects connected to the time evolution. The carrier dynamics is shown to reduce in such a way to have stringent connections to the well–known equilibrium electron–electron and electron–phonon self–energies. This link allows to use general arguments to motivate the relative balance between the e–e and e–p scattering channels on the basis of the carrier energies.

Dynamical screening effects from first principles: implications for low-energy models and application to the iron pnictides

Michele Casula[1], *Ph. Werner*[2], *F. Aryasetiawan*[3], *T. Miyake*[4,5], *L. Vaugier*[6,5], *A. Rubtsov*[7], *A. J. Millis*[8], *and S. Biermann*[6,5]

1. CNRS and Institut de Minéralogie et de Physique des Milieux Condensés, Université Pierre et Marie Curie, 4 place Jussieu, 75252, Paris cedex 05, France
2. Department of Physics, University of Fribourg, 1700 Fribourg, Switzerland
3. Department of Physics, Mathematical Physics, Lund University, Sölvegatan 14A, 22362 Lund, Sweden
4. Nanosystem Research Institute (NRI), AIST, Tsukuba, Ibaraki 305-8568, Japan
5. Japan Science and Technology Agency, CREST, Kawaguchi 332-0012, Japan
6. Centre de Physique Théorique, Ecole Polytechnique, CNRS-UMR7644, 91128 Palaiseau, France
7. Department of Physics, Moscow State University, 119992 Moscow, Russia
8. Department of Physics, Columbia University, 538 West, 120th Street, New York 10027, USA

The discovery, in 2008, of superconductivity above 50K in the iron pnictides has opened a new playground in condensed matter physics. The theoretical description of their electronic properties, even in the normal phase, poses a challenge to theory, emphasizing the need of determining many-body models entirely from first principles. A proper ab-initio derivation of low-energy correlated Hamiltonians, based on the constrained RPA method, produces a frequency dependent Coulomb interaction U, as it is dynamically screened by the higher-energy degrees of freedom. We present new methods to include these screening effects in an extended dynamical mean field theory (DMFT) framework[1, 2]. We demonstrate that the frequency dependence of U brings in additional features, such as the correlation satellites seen in photoemission spectroscopy together with a renormalization of the low-energy properties[3]. Our first application of the dynamically screened U to the iron pnictides indicates that $BaFe_2As_2$ is a strongly correlated compound with strongly doping- and temperature-dependent properties. In the hole-overdoped region an incoherent metal is found, whereas Fermi-liquid behaviour

is recovered in the undoped compound[4]. In the intermediate-doping regime, a fractional power-law behavior of the self energy is observed for the first time in a realistic modelization of materials. The resulting spectral function is in an overall agreement with the most recent ARPES data, and provides a theoretical support to their interpretation.

References

[1] Ph. Werner, and A. J. Millis, Phys. Rev. Lett. **104**, 146401 (2010).

[2] M. Casula, A. Rubtsov, S. Biermann, Phys. Rev. B **85**, 035115 (2012).

[3] M. Casula, Ph. Werner, L. Vaugier, F. Aryasetiawan, T. Miyake, A. J. Millis, S. Biermann, Phys. Rev. Lett. **109**, 126408 (2012).

[4] Ph. Werner, M. Casula, T. Miyake, F. Aryasetiawan, A. J. Millis, and S. Biermann, Nature Physics **8**, 331 (2012).

Mechanism for orbital ordering in transition-metal oxides

Eva Pavarini

Institute for Advanced Simulation and JARA-High Performance Computing

The origin of orbital order is central to the physics of many strongly-correlated transition-metal oxides. Classical examples are $KCuF_3$ and $LaMnO_3$, as well as the series of rare-earth manganites. To clarify the origin of orbital order in these paradigmatic systems, using the LDA+DMFT approach we calculate $T_{\rm KK}$, the transition temperature for the super-exchange mechanism, and disentangle the effects of super-exchange from those of lattice distortions. We show that, in all systems considered, the purely electronic super-exchange mechanism leads to remarkably high values of $T_{\rm KK}$, but cannot explain alone the persistence of orbital order up to almost the melting point [1,2,3]. Static Jahn-Teller distortions are necessary to stabilize orbital order at such high temperatures. Finally, we show that super-exchange plays a minor role in determining the orbital order-to-disorder transition observed, increasing temperature or applying pressure, in $LaMnO_3$ and in the full series of rare-earth manganites [3].

[1] E. Pavarini, E. Koch, and A.I. Lichtenstein, Phys. Rev. Lett. **101**, 266405 (2008).
[2] E. Pavarini, E. Koch, Phys. Rev. Lett. **104**, 226401 (2010).
[3] A. Flesch, G. Zhang, E. Koch, and E. Pavarini, Phys. Rev. B **85**, 035124 (2012).

Total energy and force calculations for correlated materials

Ivan Leonov

Theoretical Physics III, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany

We present an application of LDA+DMFT computational scheme for *ab initio* total energy and force calculations of materials with correlated electrons. Employing this method, it becomes possible to investigate electronic correlation effects in a solid with a given lattice structure and, most importantly, to incorporate the lattice by calculating the total energy of a correlated material as a function of the atomic positions and the unit cell. Here we employ this approach to compute the equilibrium Jahn-Teller distortion and perform a direct structural optimization of paramagnetic $KCuF_3-$ a prototypical compound in which a strong cooperative Jahn-Teller effect is known to occur. In particular, we obtained the correct lattice constant, equilibrium Jahn-Teller distortion, antiferro-orbital order, tetragonal compression of the unit cell, and spectral properties [1]. Moreover, we employed this approach to study the equilibrium crystal structure and phase stability of paramagnetic iron at the bcc-fcc phase transition [2]. For this purpose we analyzed the energetics of the bcc-fcc lattice transformation using the Bain transformation path and calculated lattice dynamical properties of paramagnetic iron as a function of temperature. Our results for the equilibrium crystal structure, phase stability, and lattice dynamics are in good quantitative agreement with experimental data. We find that electronic correlations are important to explain the lattice stability of iron at the bcc-fcc phase transition. Finally, we present our recent results obtained by the LDA+DMFT approach implemented with the linear response formalism regarding atomic displacements. Our preliminary results already show an overall good agreement between the total energy and force computations of the equilibrium atomic positions for elemental hydrogen and $SrVO_3$.

[1] I. Leonov, Dm. Korotin, N. Binggeli, V. I. Anisimov, and D. Vollhardt, Phys. Rev. B **81**, 075109 (2010).

[2] I. Leonov, A. I. Poteryaev, V. I. Anisimov, and D. Vollhardt, Phys. Rev. Lett. **106**, 106405 (2011); *idem*, Phys. Rev. B **85**, 020401 (2012).

Towards a determinant space representation of the electronic wavefunction in the solid state

George H. Booth[1,2], *Andreas Grüneis*[3], *James J. Shepherd*[2], *Georg Kresse*[3], *David P. Tew*[4], *Garnet K.-L. Chan*[1], *Ali Alavi*[2]

1. Department of Chemistry, Frick Laboratory, Princeton University, NJ, USA
2. University of Cambridge, Chemistry Department, Lensfield Road, Cambridge, UK
3. University of Vienna, Faculty of Physics and Center for Computational Materials Science, Vienna, Austria
4. School of Chemistry, University of Bristol, Bristol, UK

We have extended the Full Configuration Interaction Quantum Monte Carlo method (FCIQMC)[1, 2] to tackle both the uniform electron gas, and *ab initio* solid-state problems, providing numerically exact finite simulation-cell energies in a range of materials[3, 4]. These benchmarks are used to assess the accuracy of the established heirarchy of quantum chemical methods, up to the 'gold-standard' CCSD(T), finding almost an order of magnitude improvement in cohesive energies of simple solids compared to PBE. Limitations of these wavefunction based methods are outlined, including the basis-set convergence and the issue of excited states, and potential solutions to these discussed[5, 6].

References

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

[2] G. H. Booth, D. Cleland, A. J. W. Thom, & A. Alavi, *J. Chem. Phys.*, **135**, 084104 (2011)

[3] J. J. Shepherd, G. H. Booth, A. Grüneis, & A. Alavi, *Phys. Rev. B*, **85**, 081103 (2012)

[4] G. H. Booth, A. Grüneis, G. Kresse, A. Alavi, *Nature*, In press, (2012)

[5] G. H. Booth, D. Cleland, A. Alavi, D. P. Tew, *J. Chem. Phys.*, **137**, 164112 (2012)

[6] G. H. Booth, G. K.-L. Chan, *J. Chem. Phys.*, **137**, 191102 (2012)

Minimum energy pathways from Quantum Monte Carlo

S. Saccani[1], *C. Filippi*[2] *S. Moroni*[1],

1. SISSA and DEMOCRITOS National Simulation Center, IOM-CNR, Trieste, Italy
2. MESA+ Institute for Nanotechnology, University of Twente, Enschede, The Netherlands

We perform quantum Monte Carlo calculations to determine minimum energy pathways of simple chemical reactions, and compare the computed geometries and reaction barriers with those obtained with density functional theory and quantum chemistry methods. We find that QMC performs in general significantly better than DFT, being also able to treat cases in which DFT is inaccurate or even unable to locate the transition state. Since the wave function form employed here is particularly simple and can be transferred to larger systems, we suggest that a QMC approach is both viable and useful for reactions difficult to address by DFT and system sizes too large for high level quantum chemistry methods.

Total energy calculations: an auxiliary-field many-body perspective

Shiwei Zhang, Fengjie Ma, Wirawan Purwanto, Yudistira Virgus, Henry Krakauer, Hao Shi

Department of Physics, College of William & Mary, Williamsburg, Virginia, USA

I will discuss the auxiliary-field method as a framework for many-body total energy calculations. This is a field-theoretic approach which connects naturally to independent-electron theory, while allowing a stochastic computational implementation. As such, it is a many-body total energy method that looks like *many* coupled mean-field calculations in fluctuating external fields. Alternatively it can be thought of as a diffusion Monte Carlo calculations but with random walkers that are Slater determinants whose orbitals evolve stochastically. The constraint to remove the sign problem is formulated and carried out in Slater determinant space, which turns out to be much less restrictive and more accurate. With single-determinant constraining wave functions from Hartree-Fock or density-functional theory (DFT), this approach can be thought of as a post-DFT method with no parameter. In this form, the accuracy is typically comparable to the quantum chemistry coupled-cluster CCSD(T) method near equilibrium geometries, and better than CCSD(T) when bonds are stretched. Thus this approach combines some of the best features in key electronic structure methods: non-perturbative, high accuracy, and low-power law computational scaling with system size.
I will describe our recent progress on the calculation of excited states in solids, including the band gap in ZnO, and on further improving the accuracy of ground state calculations in transition metal systems and heavier elements. Work will also be presented on further increasing the systematic improvability of the results in strongly correlated systems by the use of symmetry and by releasing the constraint.

Predicting the Properties of Ordinary Matter Under Extreme Conditions

Jeffrey M. McMahon[1] *and David M. Ceperley*[1]

1. Department of Physics, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, USA

Recently proposed structure-prediction methods are revolutionizing our understanding of solid-state systems and becoming powerful tools in the design of novel materials. Such methods are playing a particularly important role in predicting the properties of ordinary matter under extreme pressures (and temperatures), conditions at which a significant fraction of matter exists at, for example in planetary interiors. This is because creating such conditions experimentally is extremely challenging, and thus theory and computational modeling plays the primary role in our understanding. In this talk, I will present results from the application of structure-prediction methods to two of the most abundant systems in the universe, water-ice and hydrogen. I will first discuss the ground-state structures that these systems adopt, and then go on to discuss some of the remarkable properties that they exhibit, including an insulator-to-metal transition in water-ice and high-temperature superconductivity as well as the possibility of a low- or zero-temperature quantum fluid in hydrogen.

New classes of piezoelectrics, ferroelectrics, and antiferroelectrics by first-principles high-throughput materials design

Joseph W. Bennett[1]

1. Department of Physics and Astronomy, Rutgers University, Piscataway, NJ 08854

Functional materials, such as piezoelectrics, ferroelectrics, and antiferroelectrics, exhibit large changes with applied fields and stresses. This behavior enables their incorporation into a wide variety of devices in technological fields such as energy conversion/storage and information processing/storage. Discovery of functional materials with improved performance or even new types of responses is thus not only a scientific challenge, but can have major impacts on society. In this talk I will review our efforts to uncover new families of functional materials using a combined crystallographic database/high-throughput first-principles approach. I will describe our work on the design and discovery of thousands of new functional materials, specifically the LiAlSi family as piezoelectrics, the LiGaGe family as ferroelectrics, and the MgSrSi family as antiferroelectrics.

A new generation of density-functional methods based on the adiabatic-connection dissipation-fluctuation theorem

Andreas Görling, Andreas Heßelmann, Patrick Bleiziffer

Lehrstuhl für Theoretische Chemie, Universität Erlangen-Nürnberg
Egerlandstraße 3, D-91058 Erlangen, Germany

A new generation of density-functional methods based on orbital-dependent exchange-correlation functionals is presented. The exchange energy and the local multiplicative exchange potential, not to be confused with the nonlocal Hartree-Fock exchange potential, are treated exactly. Functionals for the correlation energy are derived from the adiabatic-connection dissipation-fluctuation theorem via time-dependent density-functional theory. In the latter either the simple Coulomb kernel or the Coulomb kernel plus the full frequency-dependent exact exchange kernel is employed, leading to the correlation energy either in the straightforward random phase approximation (RPA) or in an approximation termed exact-exchange RPA (EXXRPA). In the self-consistent calculation of the orbitals the correlation potential is either neglected or treated at the RPA level. The new methods, in particular the EXXRPA approach are shown to be highly accurate and, in contrast to traditional density-functional methods, to be well-suited for the treatment of Van-der-Waals interaction or situations characterized by strong correlation.

A. Heßelmann and A. Görling, Mol. Phys.**108**, 359 (2010).
A. Heßelmann and A. Görling, Phys. Rev. Lett. **106**, 093001 (2011).
A. Heßelmann and A. Görling, Mol. Phys. **109**, 2473 (2011).
P. Bleiziffer, A. Heßelmann, and A. Görling, J. Chem. Phys. **136**, 134102 (2012).

Strong correlation in Kohn-Sham Density Functional Theory

Paola Gori-Giorgi[1], *Francesc Malet*[1]

1. Department of Theoretical Chemistry and Amsterdam Center for Multiscale Modeling, FEW, Vrije Universiteit, De Boelelaan 1083, 1081HV Amsterdam, The Netherlands

In principle, Kohn-Sham (KS) density functional theory (DFT) should yield the exact ground-state density and energy of *any* many-electron system, including physical situations in which electronic correlation is very strong, representing them in terms of *non-interacting* electrons. Currently available approximations for KS DFT, however, fail at properly describing systems approaching the Mott insulating regime, the breaking of the chemical bond, and localization in low-density nanodevices, to name a few examples. Artificially breaking the spin (or other) symmetry can mimic some (but not all) strong-correlation effects, at the price of a wrong characterization of several properties and of a partial loosening of the rigorous KS DFT framework.

In this talk, I will show how the exact strong-interaction limit of the Hohenberg-Kohn energy density functional can be used to approximate the (restriced) KS exchange-correlation energy. This corresponds to constructing a highly non-local density functional whose functional derivative (the KS potential) can be easily constructed. Otherwise said, we transform *exactly*, in a physically transparent way, an important part of the electron-electron interaction into an effective local one-body potential able to capture essential features of strong correlation that (restricted) Kohn-Sham calculations using the currently available approximations cannot describe. Open problems and future perspectives will be discussed.

Combining wave-function and density-functional theories: range-separated hybrids, multiconfigurational hybrids, and double hybrids.

Julien Toulouse

Laboratoire de Chimie Théorique, Université Pierre et Marie Curie and CNRS, Paris, France

I will present several hybrid electronic-structure calculation methods which combine wave-function and density-functional theories based on a decomposition of the electron-electron interaction:
(1) Range-separated hybrids which combine a (semi)local density-functional approximation for the long-range part of the electron-electron interaction with explicit many-body methods for the long-range part of the electron-electron interaction (see, e.g., Ref. [1]), such as second-order Møller-Plesset perturbation theory [2] or several variants of the random phase approximation [3,4,5,6,7]. This approach aims at improving the description of weak van der Waals interactions;
(2) Multiconfigurational hybrids which combine a multiconfiguration self-consistent field calculation with a (semi)local density-functional approximation [8]. This approach aims at improving the description of static (or strong) correlation;
(3) Double hybrids which combine Hartree-Fock exchange and second-order Møller-Plesset correlation with a (semi)local density-functional approximation with only one empirical parameter [9,10]. This approach aims at improving general thermochemistry properties (atomization energies, reaction barrier heights).

[1] J. Toulouse, F. Colonna, A. Savin, Phys. Rev. A 70, 062505 (2004)
[2] J. G. Angyan, I. C. Gerber, A. Savin, J. Toulouse, Phys. Rev. A 72, 012510 (2005)
[3] J. Toulouse, I. C. Gerber, G. Jansen, A. Savin, J. G. Angyan, Phys. Rev. Lett. 102, 096404 (2009)
[4] J. Toulouse, W. Zhu, J. G. Angyan, A. Savin, Phys. Rev. A 82, 032502 (2010)
[5] W. Zhu, J. Toulouse, A. Savin, J. G. Angyan, J. Chem. Phys. 132, 244108 (2010)
[6] J. G. Angyan, R.-F. Liu, J. Toulouse, G. Jansen, J. Chem. Theory Comput. 7, 3116 (2011)
[7] J. Toulouse, W. Zhu, A. Savin, G. Jansen, J. G. Angyan, J. Chem. Phys. 135, 084119 (2011)
[8] K. Sharkas, A. Savin, H. J. Aa. Jensen, J. Toulouse, J. Chem. Phys. 044104 (2012)
[9] K. Sharkas, J. Toulouse, A. Savin, J. Chem. Phys. 134, 064113 (2011)
[10] J. Toulouse, K. Sharkas, E. Bremond, C. Adamo, J. Chem. Phys. 135, 101102 (2011)

Bridging density-functional and many-body perturbation theory: orbital-density dependence in electronic-structure functionals

Andrea Ferretti[1], *Ismaila Dabo*[2], *Matteo Cococcioni*[3], *Nicola Marzari*[4]

1. Centro S3, CNR–Istituto Nanoscienze, 41125 Modena, Italy
2. Université Paris-Est, CERMICS, Projet Micmac ENPC-INRIA, 77455 Marne-la-Vallée Cedex 2, France
3. Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN 55455, USA
4. Theory and Simulations of Materials (THEOS), École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

Energy functionals which depend explicitly on the orbital densities (ODD), instead of the total charge density, appear when applying self-interaction corrections to density-functional theory. In these cases (e.g. the Perdew-Zunger [1] and the non-Koopmans [2] approaches) the total energy loses invariance under unitary rotations of the orbitals, and the minimization of the functionals leads to orbital-dependent Hamiltonians.
We show that it is possible to identify the orbital-dependency of densities and potentials with an effective and discretized frequency-dependency, in close analogy to the quasi-particle approximation of frequency-dependent self-energies and naturally oriented to interpret electronic spectroscopies [3]. Some of the existing ODD functionals are analyzed from this new perspective. Numerical results for the electronic structure of gas-phase molecules (within the Koopmans-corrected class of functionals) are computed and found in excellent agreement with photoemission (UPS) data [4].

[1] J.-P. Perdew and A. Zunger, Phys. Rev. B **23**, 5048 (1981).
[2] I. Dabo, A. Ferretti, N. Poilvert, Y. Li, N. Marzari, M. Cococcioni, Phys. Rev. B **82**, 115121 (2010).
[3] M. Gatti, V. Olevano, L. Reining, I.-V. Tokatly, Phys. Rev. Lett. **99**, 057401 (2007).
[4] I. Dabo, A. Ferretti, C.-H. Park, N. Poilvert, Y. Li, M. Cococcioni, N. Marzari, Phys. Chem. Chem. Phys. in press (2012, DOI 10.1039/C2CP43491A).

TITLES OF

ABSTRACTS

OF

POSTERS

Key to Main Topics

Theory and Methods:

T1 Density-Functional Theory beyond LDA
T2 Time Dependent DFT
T3 Many-Body Techniques for Real Materials
T4 Quantum Monte Carlo
T5 Ab-initio Molecular Dynamics
T6 Large-Scale and Multiscale Simulations
T7 Activated Processes
T8 Electronic and Thermal Transport
T9 Response to External Fields
T10 Simulations in Realistic Environments
T11 Other methods

Applications:

A1 Nanoscience
A2 Biochemistry and Biomaterials
A3 Magnetism and Spintronics
A4 Geophysics
A5 Functional Materials
A6 Surfaces
A7 Spectroscopies
A8 Catalysis and Electrochemistry
A9 Chemical Reactions and Kinetics
A10 Materials Design
A11 Other applications

POSTER SESSION 1

THURSDAY 10 JANUARY 2013

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

http://cdsagenda5.ictp.it/full_display.php?ida=a12161

POSTER SESSION I

THURSDAY 10 JANUARY 2013

In alphabetical order of presenting author (underlined)

Electronic structure of Co doped ZnO from the GW perspective

I. Abdolhosseini Sarsari [12], C. Das Pemmaraju[2], Hadi Salamati[1], Stefano Sanvito[2]
1. Department of Physics, Isfahan University of Technology, Isfahan, 84156- 83111, Iran 2. School of Physics and CRANN, Trinity College, Dublin 2, Ireland
T3

The true role of many-body polarization forces in describing the properties of liquid water

Omololu Akin-Ojo[1] and Krzysztof Szalewicz[2]
1. African University of Science and Technology, Abuja, NIGERIA 2. University of Delaware, Newark, DE, USA
T5

Dispersion interactions in DFT and linear-scaling DFT

Lampros Andrinopoulos[1], Nicholas D. M. Hine[1], Arash A. Mostofi[1]
1. Imperial College London
T1

Theoretical studies on a gramicidin A channel using a linear-scaling DFT technique

M. Arita[1,2], M. Todorovic[3], W. Shinoda[4], D.R. Bowler[5] and T. Miyazaki[2,1]
1. Department of Physics, Tokyo University of Science, Japan 2. Computational Materials Science Unit, National Institue for Materials Science, Japan 3. Departamento de Fisica Teorica de la Materia Condensada, Universidad Autonoma de Madrid, Madrid, Spain 4. Advanced Health Research Group, Advanced Industrial Science and Technology, Japan 5. Department of Physics & Astronomy, University College London, UK
T6

Structure of liquid water from first-principles simulations with van der Waals interactions

F. Corsetti[1], E. Artacho[1,2], J. M. Soler[3], M.-V. Fern´andez-Serra[4]
1CIC nanoGUNE Consolider, 20018 Donostia-San Sebasti´an, Spain 2Dept. of Physics, University of Cambridge, Cambridge CB3 0HE, United Kingdom 3Dept. de F´ısica de la Materia Condensada, Universidad Autonoma de Madrid, 28049 Madrid, Spain 4Dept. of Physics and Astronomy, Stony Brook University, Stony Brook, New York 11794-3800, USA
T5

Reaction pathways and structural properties by Quantum Monte Carlo

Matteo Barborini[1,2], Leonardo Guidoni[2]
1. Dipartimento di Matematica Pura ed Applicata, Universita` degli studi dell'Aquila, via Vetoio (Coppito 2), 67100 L'Aquila, Italy 2. Dipartimento di Scienze Fisiche e Chimiche, Universita` degli studi dell'Aquila, via Vetoio (Coppito 2), 67100 L'Aquila, Italy
T4

Electronic and Optical properties of ZnO Quantum Dots, Nanorods and Nanoflakes: an atomistic study

Zaiping Zeng1, C. S. Garoufalis1, S. Baskoutas1 and G. Bester2
1. Materials Science Department, University of Patras, Greece
2. Max-Planck Institute for Solid State Research, Stuttgart, Germany
T11

FHI-aims becomes embedded: a full-potential QM/MM approach

Daniel Berger 1 Volker Blum 2 Karsten Reuter 1
1 TU Munchen, Lichtenbergstrae 4, 85747 Garching
2 FHI, Faradayweg 4-6, 14195 Berlin
T6

Are Polarization and Magnetization Really Bulk Properties?
Raffaello Bianco[1], Raffaele Resta[1,2]
1. Dipartimento di Fisica, Universita di Trieste
2. CECAlvI, Ecole Polytechnique Federale de Lausanne, Switzerland
T9

Orbital density dependent functionals: a powerful tool for electronic structure calculations
Giovanni Borghi[1], Linh Nguyen[1], Andrea Ferretti[2], Cheol-Hwan Park[3], Nicolas Poilvert[4], Ismaila Dabo[5], Nicola Marzari[1]
1. Ecole Polytechnique F´ed´erale de Lausanne 2. CNRNANO, Universita di Modena e Reggio Emilia 3. Department of Physics and Astronomy, Seoul National University 4. Department of Materials Science and Engineering, Massachusset's Institute of Technology. 5. CERMICS, Universite Paris-Est
T1

Range-separated approach to the RPA correlation applied to van der Waals bond and to diffusion of defects
Fabien Bruneval[1],
1. CEA, DEN, Service de Recherches de M´etallurgie Physique, F-91191 Gif-sur-Yvette, France
T1

Variational approach to hydrogen's electronic structure
Francesco Calcavecchia, Thomas Kuhne
Institut fur Physikalische Chemie, Johannes Gutenberg University, Mainz
T11

Comparison of stress and total energy methods for the calculation of elastic properties of semiconductors
Miguel A. Caro[1,2], Stefan Schulz[1], Eoin P. O'Reilly[1,2]
1. Tyndall National Institute, Dyke Parade, Cork City, Ireland 2. Department of Physics, University College Cork, Cork, Ireland
T9

Epinephrine geometrical parameters study using car-parrinello molecular dynamics
Arsênio P. Vasconcelos-Neto[1], Valter H. C. Silva[2], Nayara D. Coutinho[3] , Ademir J. Camargo[4]
T5

Thermal conductivity and expansion of crystals from first principles
A. Cepellotti[1], N. Bonini[2], N. Marzari[1]
1. Theory and Simulation of Materials, Ecole Polytechnique Federale de Lausanne, 1007 Lausanne, Switzerland 2. Department of Physics, King's College London, London WC2R 2LS, United Kingdom
T8

Wannier Functions study of chemical bonds in B12 and B28
D. Ceresoli and C. Gatti
Institute of Molecular Science and Technology (ISTM), CNR, Milan, Italy
T11

Defect Ordering in hard PbTiO3
Anand Chandrasekaran[1,2], Dragan Damjanovic[2], Nava Setter[2] Nicola Marzari[1],
1. Theory and Simulation of Materials, École Polytechnique Fédérale de Lausanne 2. Ceramics Laboratory, École Polytechnique Fédérale de Lausanne
T7

Protein field effect on the dark state of 11-cis Retinal in Rhodopsin by Quantum Monte Carlo
Emanuele Coccia[1], Daniele Varsano[2], Leonardo Guidoni[1]
1. Dipartimento di Scienze Fisiche e Chimiche, Universit degli Studi dellAquila, via Vetoio, 67100, LAquila, Italy 2. Dipartimento di Fisica, Sapienza - Universita di Roma, piazzale Aldo Moro 5, 00185, Rome, Italy
T4

New implementations of the orbital minimization method in the SIESTA code
F. Corsetti1, E. Artacho1,2, G. Huhs3, R. Grima3, J. M. Cela3
1CIC nanoGUNE Consolider, 20018 Donostia-San Sebastian, Spain 2Dept. of Physics, University of Cambridge, Cambridge CB3 0HE, United Kingdom 3Barcelona Supercomputing Center-Centro Nacional de Supercomputacion, 08034 Barcelona, Spain
T6

Study of the hydration effect on the carbamazepine geometric parameters using the Car-Parrinello molecular dynamic
Wesley P. Barbosa1, Nayara D. Coutinho1, Valter H. C. Silva2, Arsênio P. V.Neto1, Ademir J. Camargo1
1. State University of Goias 2. University of Brasilia
T5

Adsorption of Small Molecules at Kaolinite: a van der Waals DFT study
Loic Roch1, Stephen J. Cox1 and Angelos Michaelides1
1. Thomas Young Centre, London Centre for Nanotechnology and Department of Chemistry, University College London, United Kingdom
T1

Differential polarization effects with wave function/DFT embedding for excited states
Csaba Daday1, Johannes Neugebauer2, Claudia Filippi1
1. MESA+ Institute for Nanotechnology, University of Twente, The Netherlands 2. Theoretical Organic Chemistry, University of Munster, Germany
T6

Structure and Thermochemistry of Borosilicate Glass
Peter Kroll, Atreyi Dasmahapatra
Department of Chemistry and Biochemistry, The University of Texas at Arlington, USA
T5

Second Order Møller-Plesset Perturbation Theory and Random Phase Approximation Correlation Energies with Resolution-of-Identity Approximation: An Efficient and Massively Parallel Gaussian and Plane Waves Approach
Mauro Del Ben1, Jurg Hutter1, Joost VandeVondele2 1. Institute of Physical Chemistry, University of Zurich 2. Department of Materials, ETH Zurich
T1

Diffusion Monte Carlo for Heavy Atoms
René Derian[1], Shi Guo[2] ,Lubos Mitas[2]
1.Institute of Physics, Slovak Academy of Sciences, Dúbravská cesta 9, Bratislava, SK-845 11, Slovakia
2. North Carolina State University, 851 Main Campus Drive, Partners III, Raleigh, NC 27695, USA
T4

A First Principles Approach to Thermal Transport in Nanomaterials
Giorgia Fugallo,1 Michele Lazzeri,1 Lorenzo Paulatto,1 and Francesco Mauri1
1IMPMC, Universite Pierre et Marie Curie, CNRS, 4 place Jussieu, F-75252 Paris, France
T8

Electronic transport properties of grain boundaries in graphene
Fernando Gargiulo1, Oleg V. Yazyev1
1. Institute of Theoretical Physics, Ecole Polytechnique Fdrale de Lausanne (EPFL), Switzerland
T8

Exciton dispersion from first principles
Matteo Gatti1,2, Pierluigi Cudazzo3,2, Angel Rubio3,2, Francesco Sottile1,2
1. LSI, CNRS, Ecole Polytechnique, 91128 Palaiseau (France) 2. European Theoretical Spectroscopy Facility (ETSF) 3. UPV/EHU San Sebastian (Spain)
T3

Why is water difficult for DFT?
An analysis using GAP potentials and quantum Monte Carlo
M. J. Gillan 1,3,4, D. Alfè2,3,4, A. Bartók5, G. Csányi5
London Centre for Nanotechnology, UCL, London WC1H 0AH, UK
Dept. of Earth Sciences, UCL, London WC1E 6BT, UK
Dept. of Physics and Astronomy, UCL, London WC1E 6BT, UK
Thomas Young Centre at UCL, London WC1E 6BT, UK
Dept. of Engineering, University of Cambridge, Cambridge CB2 1PZ, UK
T11

Implementation of the image charge method in QM/MM
Dorothea Golze, Marcella Iannuzzi, Jurg Hutter
University of Zurich, Winterthurerstr. 190, CH-8057 Zurich, Switzerland
T6

Efficient relativistic nuclear magnetic resonance J-coupling with pseudopotentials and the zeroth-order regular approximation
Timothy F. G. Green[1], Jonathan R. Yates[1]
1. Department of Materials, University of Oxford
T9

First-principles calculation of Seebeck coefficient of $AgSbSe_2$
Shima Sharifi [1], Seyed Javad Hashemifar [1], Hadi Akbarzadeh [1]
1. Dep. of Physics, Isfahan University of Technology, 8415683111 Isfahan, Iran
T8

Study of Vanadium- and Cobalt-Benzene Half-Sandwich Arenes by Stochastic Quantum Sampling Approach
L.Horváthová1, Matúš Dubecký 1, I. Štich 1 ,L. Mitas, 2
1. Institute of Physics, Center for Computational Materials Science, Slovak Academy of Sciences, 845 11 Bratislava, Slovakia 2. Department of Physics and CHiPS, North Carolina State University, Raleigh, NC 27695
T4

Performance of local orbital basis sets in the self-consistent Sternheimer method for dielectric screening of extended systems
Hannes Hubener,[1] Miguel Angel Perez-Osorio,[2] Pablo Ordejon[2] and Feliciano Giustino[1]
1. Department of Materials, University of Oxford, Oxford OX1 3PH, United Kingdom 2. Centre d'Investigacio en Nanociencia i Nanotecnologia-CIN2 (CSIC-ICN), Bellaterra, Spain
T3

The GW approximation in GPAW
Falco Huser[1], Kristian Sommer Thygesen
1. Center for Atomic-scale Materials Design, Technical University of Denmark
T3

Enhanced metallicity in armchair graphene nanoribbons with Cu impurities
Neeraj K. Jaiswal and Pankaj Srivastava
Nanomaterials Research Group, Computational Nanoscience and Technology Lab. (CNTL) ABV- Indian Institute of Information Technology and Management, Gwalior- 474015, India
T8

Quasi-linear band structure and electronic transport in transparent conducting oxides
Youngho Kang[1], Seungwu Han[1]
1. Department of Materials Science and Engineering, Seoul National University, Seoul 151-744, Korea
T8

Radiation damage in biological systems: Ab initio MD studies
Maeve Smyth[1], Jorge Kohanoff[1],
1.Atomistic Simulation Centre, Queen's University Belfast, Northern Ireland, UK
T10

Electronic correlations and crystal structure distortions in BaBiO3
Dm. Korotin[1], V. Kukolev[2], A. V. Kozhevnikov[3] D. Novoselov[1] V. I. Anisimov[1,4]
1. Institute of Metal Physics, S. Kovalevskoy St. 18, 620990 Yekaterinburg, Russia 2. Ural State University, Pr. Lenina 51, 620083 Yekaterinburg, Russia 3. Institute for Theoretical Physics, ETH Zurich, CH-8093 Zurich, Switzerland 4. Ural Federal University, 620002 Yekaterinburg, Russia
T1

Magnetic Spectroscopies with DFT + Hubbard (U,V)
E. Kucukbenli[1,2] N. Marzari[1]
1. Ecole Polytechnique Federale de Lausanne, Switzerland
2. CNR-IOM Democritos, Italy
T9

Infulence of exchane-correlation functional on local order competition in disordered phase of Ge2Sb2Te5: octahedral versus tetrahedral Ge
Kye Yeop Kim, Seungwu Han†
Department of Materials Science and Engineering, Seoul National University, Seoul, Korea, 151-744
T1

Ab-initio Sternheimer-GW method for quasiparticle calculations
Henry Lambert and Feliciano Giustino
Department of Materials, University of Oxford, Parks Road, Oxford, OX1 3PH, United Kingdom
T3

Strongly-correlated quantum wires within Kohn-Sham Density Functional Theory
Francesc Malet[1], Paola Gori-Giorgi[1], and Jonas C. Cremon[2]
1.Department of Theoretical Chemistry and Amsterdam Center for Multiscale Modeling, Vrije Universiteit, 1181 HV Amsterdam, The Netherlands. 2.Mathematical Physics, LTH, Lund University, SE-22100 Lund, Sweden
T1

Disorder effects in solid state systems beyond a single-site prospective: theories and applications
Alberto Marmodoro[1], Arthur Ernst[2] 1. Max-Planck-Institut fur Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany
T11

Efficient evaluation of Fock exchange for non-localized wave-functions
Margherita Marsili[1], Paolo Umari[1]
1. Dipartimento di Fisica e Astronomia 'Galileo Galilei' – Università degli Studi di Padova, Via Marzolo 8, 35131 Padova - Italy
T1

Polyamorphism in CO2 from ab initio molecular dynamics
Dušan Plašienka, Roman Martoňák
Department of Experimental Physics, Faculty of Mathematics, Physics and Informatics, Comenius University, Mlynská dolina F2, 842 48 Bratislava, Slovakia
T5

Z-method calculation of the Mg melt curve
Shailesh Mehta1
AWE Aldermaston, Reading, RG7 4PR, United Kingdom
T5

Structural and orbital phase transitions induced by Jahn-Teller distortions in KCuF3
Joaquin Miranda*, Erik Koch* and Eva Pavarini**
*German Research School for Simulation Sciences, Forschungszentrum Jülich and RWTH Aachen University, 52425 Jülich
**Institute for Advanced Simulation and JARA, Forschungszentrum Jülich
T11

Extension of the SCE Formalism to Fractional Electron Numbers and Investigation of the Derivative Discontinuity

A. Mirtschink[1], M. Seidl[2], P. Gori-Giorgi[1]
1. Department of Theoretical Chemistry and Amsterdam Center for Multiscale Modeling, FEW, Vrije Universiteit, De Boelelaan 1083, 1081HV Amsterdam, The Netherlands 2. Institute of Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany

T1

Doping at the Si-SiO2 interface

Fabiano Corsetti[1], Arash Mostofi[2]
1. CIC nanoGUNE Consolider, Donostia-San Sebastian, Spain 2. Departments of Materials and Physics, and the Thomas Young Centre for Theory and Simulation of Materials, Imperial College London, London, UK

T6

Topological surface state scattering in Antimony

Awadhesh Narayan[1], Ivan Rungger[1], Stefano Sanvito[1]
1. School of Physics and CRANN, Trinity College Dublin, Ireland.

T8

Spin transport and magnetic behavior of boron nitride nanoribbons with magnetic impurities

George Alexandru Nemnes1, Tudor Luca Mitran1, Adela Nicolaev1, Lucian Ion1, Stefan Antohe1
1. University of Bucharest, Faculty of Physics, "Materials and Devices for Electronics and Optoelectronics" Research Center

T8

Photoemission spectroscopy from Koopmans' compliant functionals, and its application to the tautomeric populations of DNA and RNA nucleobases

Ngoc Linh Nguyen[1], Giovanni Borghi[1], Andrea Ferretti[2], Ismaila Dabo[3], Nicola Marzari[1]
1. Theory and Simulation of Materials (THEOS), Ecole Polytechnique Federale de Lausanne 2. CNRNANO, Universita di Modena e Reggio Emilia 3. CERMICS, Universite Paris-Est

T1

Spin state transition in LaCoO3: a DFT+DMFT aproach

Novoselov D.[1], Anisimov V.I.[1]
1. Institute of metal physics, Ural Branch, Russian Academy of Sciencies

T4

Frequency-dependent Hubbard U corrections to DFT: A simple approach

David D. O'Regan, Nicola Marzari
Theory and Simulation of Materials, Ecole Polytechnique Federale de Lausanne

T3

Extending the random-phase approximation for electronic correlation energies: The renormalized adiabatic local density approximation

Thomas Olsen1 and Kristian S. Thygesen1
1. Center for Atomic-Scale Materials Design (CAMD) and Center for Nanostructured Graphene (CNG), Department of Physics, Technical University of Denmark

T1

Wavelets and Projector Augmented-Wave approach: an adaptive basis set for large-scale calculations at all-electron accuracy

T. Rangel[1], M. Torrent[1]
1. CEA, DAM, DIF, F-91297 Arpajon, France

T6

A new field-theoretic approach to linear scaling ab-initio molecular dynamics

Dorothee Richters, Thomas D. Kuhne
Institute for Physical Chemistry, University of Mainz, Germany

T5

Optical Absorption in B−19 Cluster : A Time Dependent Density Functional Approach
Ravindra Shinde, Alok Shukla
Department of Physics, Indian Institute of Technology Bombay, Mumbai, Maharashtra 400076, India
T2

Recent progress in the theory of flexoelectric response
Massimiliano Stengel[1,2]
1. ICMAB-CSIC, Campus UAB, 09193 Bellaterra, Spain 2. ICREA - Institucio´ Catalana de Recerca i Estudis Avan çats, 08010 Barcelona, Spain
T9

Strong Isotope effect in phase II of Dense Solid Hydrogen and Deuterium
Gregory Geneste, Marc Torrent, Francois Bottin and Paul Loubeyre
CEA, DAM, DIF. F-91297 Arpajon. France
T5

Computer simulation of the reaction mechanism of matrix metaloprotease MMP3 by QM/MM methods
Marcelo Adrian Martí[1], Gustavo Troiano Feliciano[2], Antonio José Roque da Silva[3]
1. Departamento de Química Biológica e INQUIMAE-CONICET, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires, Ciudad Universitaria, Pabellón 2, Buenos Aires, C1428EHA, Argentina.
2. Centro de Ciências Naturais e Humanas, Departamento de Ciência e Tecnologia Química – Universidade Federal do ABC- UFABC- Santo Andre, SP, Brazil
3. Departamento de Física dos Materiais e Mecânica, Instituto de Física, Universidade de São Paulo, SP, Brasil
T6

Towards Petascale DFT-calculations: a new parallelization approach for linear response and exact exchange
Nicola Varini
iVEC, 26 Dick Perry Ave,Kensington WA 6151, Australia
T6

Kohn-Sham orbitals from Quantum Monte Carlo Density
Daniele Varsano[1], Matteo Barborini[2] and Leonardo Guidoni[3]
1. Department of Physics, Sapienza Universita di Roma, Italy 2. Department for Pure and Applied Mathematics, Univesity of l'Aquila, Italy 3. Department of Chemistry, Chemical Engineering and Materials, Univesity of l'Aquila, Italy
T4

Ab initio angle- and energy-resolved photoelectron spectroscopy with time-dependent density-functional theory
Umberto De Giovannini[1], Daniele Varsano[2], Miguel A. L. Marques[3], Heiko Appel[4], Ebherard K. U. Gross [5] and Angel Rubio [1]
1. University of the Basque Country UPV/EHU, Nano-Bio Spectroscopy Group, Spain 2. Department of Physics, Sapienza University of Rome, Roma, Italy 3. University of Lyon and LPMCN, CNRS France
4. Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany 5. Max-Planck Institute for Microstructure Physics, Halle, Germany
T2

Effective Hamiltonians for large-scale ab-initio lattice dynamics simulations of perovskites and related materials
Jacek C. Wojdel, Mathias Ljungberg, Jorge Inıguez
Institut de Ciencia de Materials de Barcelona (ICMAB-CSIC), Campus UAB, 08193 Bellaterra, Spain
Patrick Hermet, Philippe Ghosez
Department of Physics, University of Liege, B-4000 Sart-Tilman, Belgium
T6

Calculation of thermoelectric properties from first-principles

Bin Xu[1], Matthieu Verstraete[1]
1. Department of Physics, University of Liege, B-4000 Sart Tilman, Belgium

T8

Optimized Structure and Vibrational Properties by Error Affected Potential Energy Surfaces

Zen Andrea[1], Delyan Zhelyazov[2], Matteo Barborini[2], Sandro Sorella[3] Leonardo Guidoni[2]
1. Dipartimento di Fisica, La Sapienza - Universita` di Roma, P.le Aldo Moro 2, 00185 Roma, Italy 2. Dipartimento di Chimica, Ingegneria Chimica e Materiali, Universita` degli studi dell'Aquila, Localita` Campo di Pile, 67100 L'Aquila, Italy
3. Scuola Internazionale Superiore di Studi Avanzati (SISSA), via Bonomea 265, 34136 Trieste, Italy

T4

POSTER SESSION II

FRIDAY 11 JANUARY 2013

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

http://cdsagenda5.ictp.it/full_display.php?ida=a12161

POSTER SESSION II

FRIDAY 11 JANUARY 2013

In alphabetical order of presenting author (underlined)

Thermal and electrical conductivity of iron and iron alloys at Earth's core conditions

Monica Pozzo[1], Chris Davies[2], David Gubbins[1,2] and Dario Alfè[1]
1. Department of Earth Sciences and Thomas Young Centre @ UCL, Department of Physics and Astronomy and London Centre for Nanotechnology University College London, Gower Street, WC1E 6BT, London, U.K
2. School of Earth and Environment, University of Leeds, Leeds LS2 9JT, UK
3. Institute of Geophysics and Planetary Physics, Scripps Institution of Oceanography, University of California at San Diego, 9500 Gilman Drive #0225, La Jolla, CA 92093-0225
A4

Dielectric Properties of Functional Oxide thin-films from First Principles

J. Alsaei[1], Neil Alford[2], Paul Tangney[1], Arash A. Mostofi[1]
1. Departments of Materials and Physics, Imperial College London, SW7 2AZ, United Kingdom.
2. Department of Materials, Imperial College London, SW7 2AZ, United Kingdom.
A5

A mechanism for the α-ǫ phase transition in Iron.

Bertrand Dupe, Bernard Amadon , Yves-Patrick Pellegrini and Christophe Denoual
CEA, DAM, DIF, F 91297 Arpajon, France
A11

Ab initio study of the nucleation of Ge dimers on the {105} facets of a Ge hut

Sergiu Arapan[1], David Bowler[2], Tsuyoshi Miyazaki[1]
1. Computational Materials Science Unit, National Institute for Materials Science, Tsukuba, Japan 2. Department of Physics and Astronomy, University College London, UK
A1

Edge functionalization of zigzag graphene nanoribbons with sodium

Ozan Arı, İbrahim Dursun and R. Tuğrul Senger
Department of Physics, İzmir Institute of Technology, 35430 İzmir
A1

Layered Cobalt Oxides for Oxygen Evolution Reaction

Michal Bajdich[1,3], Mónica García-Mota[2], Jens K. Nørskov[2] and Alexis T. Bell[3,1]
1 JCAP-North, The Joint Center for Artificial Photosynthesis, Lawrence Berkeley National Laboratory, Berkeley, California 94720, United States
2SUNCAT Center for Interface Science and Catalysis, Department of Chemical Engineering, Stanford University, Stanford, California 94305, United States
3 Department of Chemical and Biomolecular Engineering, University of California at Berkeley, Berkeley, California 94720, United States
A8

First principles calculations of electronic structure and magnetic properties of the III-VI diluted magnetic semiconductor $In_{1-x}Mn_xS$

H.Ben Abdallah[1], R.Bennaceur[2]
1. Laboratoire de Phsique de la Matière Condensée, Département de Physique, Faculté des Sciences de Tunis. Tunisia
2. Laboratoire de Phsique de la Matière Condensée, Département de Physique, Faculté des Sciences de Tunis. Tunisia
A3

The study of displacive phase transitions in $SrTiO_3$-$PbTiO_3$ oxide superlattices using first principles all-atom effective Hamiltonians

Nicholas Bristowe[1], Jinzhu Zhao[1], Jacek Wojdel[2], Jorge Íñiguez[2], Philippe Ghosez[1]
1. Department of Physics, University of Liège, B-4000 Sart-Tilman, Belgium 2. Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Campus UAB, E-08193 Bellaterra, Spain

A5

Ab initio study of ZnO-based interfaces for photovoltaic applications: from hybrid to fully inorganic heterostructures

Arrigo Calzolari[1], Alice Ruini[1,2], Alessandra Catellani[1]
1 CNR-NANO Istituto Nanoscienze, Centro S3, Modena Italy
2 Dip. Fisica, Università di Modena e Reggio E., Modena Italy

A1

Electronic localization and magnetism in intermetallic alloys from ab initio calculations

Matteo Cococcioni and Burak Himmetoglu
Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN, USA

A3

Ab-initio phonon dispersions of transition and noble metals: effects of the exchange and correlation functional.

A. Dal Corso[1,2] 1. International School for Advanced Studies, SISSA, Trieste, Italy
2. CNR-IOM DEMOCRITOS Simulation Centre, Trieste, Italy

A7

Phonon dispersions in iron: embedded atom potentials, first-principles calculations, and experimental results

Daniele Dragoni, Davide Ceresoli, and Nicola Marzari
Ecole Polytechnique Federale de Lausanne

A7

Catalytic Reduction of SO2 by CO over PtlAum(CO)n: A First-principles Investigation

Guo-Ping Gao, Shi-Hao Wei Xiang-Mei Duan,
Department of Physics, Faculty of Science, Ningbo University, Ningbo-315211, P.R. China

A8

Magnetism in thiolated gold model junctions

Matus Dubecky1, Haibin Su2
1.Department of Physical Chemsitry. Palacky University in Olomouc, Bratislava, Slovakia
2. Division of Materials Science, Nanyang Technological University, Singapore

A3

Anharmonic effects from the self-consistent harmonic approximation: the example of simple cubic calcium

Ion Errea[1,2]
1. Institut de Minéralogie et de Physique des Milieux Condensés (IMPMC), Université Pierre et Marie Curie (UPMC), Case 115, 4 Place Jussieu, 75252, Paris Cedex 05, France 2. IKERBASQUE, Basque Foundation for Science, 48011, Bilbao, Spain

A7

Charge Localization Dynamics Induced by Oxygen Vacancies on the TiO2(110) Surface and Titania and Gold-promoted Titania Surfaces

Matteo Farnesi Camellone, Dominik Marx
Lehrstuhl fur Theoretische Chemie, Ruhr–Universitat Bochum, 44780 Bochum, Germany

A6

Quasiparticle band gaps of metal chalcogenides of the stibnite family for semiconductor-sensitized solar cells

Marina R. Filip, Christopher E. Patrick, and Feliciano Giustino
Department of Materials, University of Oxford, Parks Road, Oxford, OX1 3PH, United Kingdom

A5

Theory and first principle calculation of CVV Auger spectra of magnetic systems

Guido Fratesi[1], Mario Italo Trioni[2], and Gian Paolo Brivio[1] 1. Dipartimento di Scienza dei Materiali, Milano-Bicocca, Milano, Italy
2. CNR-ISTM, Milano, Italy

A7

Density functional simulations of Sb-rich GeSbTe phase change alloys

Silvia Gabardi1, Sebastiano Caravati2, Marco Bernasconi1, Michele Parrinello2
1. Dipartimento di Scienza dei Materiali, Universita di Milano-Bicocca, Via R. Cozzi 53, I-20125, Milano, Italy
2. Department of Chemistry and Applied Biosciences, ETH Zurich and Facolta` di Informatica, Istituto di Scienze Computazionali, Universita della Svizzera Italiana, Via Giuseppe Buffi 13, 6900 Lugano, Switzerland

A5

Towards a Complete and Reliable Pseudopotential Library: PAW vs All-Electron Across the Periodic Table

X. Ge,[1] B. I. Adetunji,[3,4,1] M. Monni,[5] E. Kucukbenli,[6] A. Dal Corso,[1,2] S. de Gironcoli[1,2]
1. International School for Advanced Studies, SISSA, Trieste, Italy 2. CNR-IOM DEMOCRITOS Simulation Centre, Trieste, Italy 3. Department of Physics, University of Agriculture, Abeokuta, Nigeria 4. Abdus Salam International Centre for Theoretical Physics, Trieste, Italy 5. CNR-IOM SLACS Laboratory, Cagliari, Italy 6. Ecole Polytechnique Federale de Lausanne (EPFL), Lausanne, Switzerland

A10

Electron-hole puddles in the absence of charged impurities

Marco Gibertini[1,2], Andrea Tomadin[1], Francisco Guinea[3], Michail I. Katsnelson[4], and Marco Polini[1]
1. NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore, I-56126 Pisa, Italy 2. Theory and Simulation of Materials, E`cole Polytechnique F´ed´erale de Lausanne, CH-1015 Lausanne, Switzerland
3. Instituto de Ciencia de Materiales de Madrid (CSIC), Sor Juana Ines de la Cruz 3, E-28049 Madrid, Spain 4. Radboud University Nijmegen, Institute for Molecules and Materials, NL-6525 AJ Nijmegen, The Netherlands

A1

Adsorption of Pentacene on Palladium(100) Surface – A Theoretical Study

Govindarajan Saranya, P. Kolandaivel and K. Senthilkumar*
Department of Physics, Bharathiar University, Coimbatore - 641 046, India

A6

Nonlinear dielectric effects in solvation models: Applications to dendrite formation in Lithium batteries

Deniz Gunceler1, Kathleen Schwarz2, Ravishankar Sundararaman1, Kendra Letchworth-Weaver1, T. A. Arias1
1. Department of Physics, Cornell University 2. Department of Chemistry and Chemical Biology, Cornell University

A6

Phonon Dispersions, Electronic Structure and Photocatalytic Properties of X-doped (X=N, B and Pt) Rutile TiO2 from Density Functional Theory

Sanjeev K. Gupta1,2, Igor Lukačević3 and Prafulla K. Jha2
1Department of Physics, Maharaja Krishnakumarsinhji Bhavnagar University, Bhavnagar-364001, India
2Department of Physics, Michigan Technological University, Houghton, Michigan 49931, USA 3Department of Physics, University J. J. Strossmayer, Osijek, Croatia

A7

Clustering and Diffusion of Hydrogen in α-Fe Including Quantum Effects
Erin Hayward1, Chu Chun Fu1
1. CEA-Saclay, DEN, Service de Recherches de Metallurgie Physique, Gif-sur-Yvette, France
A10

***Ab Initio* Study of Magnetic Anisotropy Energy of Some Low Dimensional Systems**
Mighfar Imam1, 2, Shobhana Narasimhan2
1. The Abdus Salam International Centre for Theoretical Physics, Strada Costiera 11, Trieste 34151, Italy. 2. Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur 560064, Bangalore, India
A3

Substrate and chemical functionalization induced magnetic moment on hexagonal boron nitride
Niharika Joshi1 and Prasenjit Ghosh2
1. Department of Physics, Indian Institute of Science Education and Research, Pune, India 2. Department of Physics and Chemistry, Indian Institute of Science Education and Research, Pune, India
A3

***Ab Initio* Study of the Adsorption of NO on small Rh clusters supported on MgO**
Bulumoni Kalita**,** Shobhana Narasimhan
Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur 560064, Bangalore, India
A8

Study of Structural, Electronic and Magnetic Properties of Pd_n, Pd_nMn_1 and Pd_nMn_2 clusters
G. C. Kaphle1,2, N. P. Adhikari1 and A. Mookerjee2
1Central Department of Physics, Tribhuvan University, Kirtipur, Kathmandu, Nepal
2Department of Condensed Matter and Materials Science, S N Bose National Centre for Basic Sciences, Block JD, Sector III, Salt Lake, Kolkata 700098, India
A3

Study of Al/Al2O3 Interface with Reactive Force Field
Manana Koberidze1, Risto M. Nieminen2
1. Aalto Univerisy, School of Science, Department of Applied Physics
2. Aalto Univerisy, School of Science, Department of Applied Physics
A6

Electrocaloric effect in ferroelectric alloys from atomistic simulations
S. Lisenkov*, I. Ponomareva
Department of Physics, University of South Florida, Tampa, USA
A5

EELS Signature of Boron Nitride Nanoribbons
Charlotte I. Lynch1, Rebecca J. Nicholls1, Timothy J. Pennycook2, Peter D. Nellist1, Jonathan R. Yates1
1. Department of Materials, University of Oxford, Parks Road, Oxford, OX1 3PH, United Kingdom 2. SuperSTEM Laboratory, STFC Daresbury, Keckwick Lane, Warrington, WA4 4AD, United Kingdom
A1

Role of pyridine derivatives on the electronic properties of polymer/metaloxide interfaces for photovoltaics
Giuliano Malloci 1 and Alessandro Mattoni 1
1. Istituto di Officina dei Materiali del CNR, SLACS Unita` di Cagliari, c/o Dipartimento di Fisica, Cittadella Universitaria S.P. Monserrato-Sestu Km 0.700, I-09042 Monserrato (CA) - ITALY
A1

Study of nanoconfinement of O_2 molecules in fullerenes and nanotubes
Daniel V P Massote1, Mário S C Mazzoni1
1. Universidade Federal de Minas Gerais, Physics Department - Brazil
A1

DFT-based ΔSCF: An efficient alternative for isomerization dynamics of adsorbed molecular switches?!

Reinhard J. Maurer, Karsten Reuter
Lehrstuhl für Theoretische Chemie, Technische Universität München

A1

Anderson localization in crystalline phase-change materials

W. Zhang1, A. Thiess2, P. Zalden3, R. Zeller2, P. H. Dederichs2,
J.-Y. Raty4, M. Wuttig3,5, S. Blugel2,5, and R. Mazzarello1,5
1 Institut fur Theoretische Festkorperphysik, RWTH Aachen University, D-52056 Aachen, Germany 2 Peter Grunberg Institut and Institute for Advanced Simulations, Forschungszentrum Julich, D-52425 Ju¨lich, Germany 3 I. Physikalisches Institut (IA), RWTH Aachen University, D-52056 Aachen, Germany 4 Physique de la Matiere Condensee, B5, Universite de Liege, B4000 Sart-Tilman, Belgium 5 JARA, RWTH Aachen University, D-52056 Aachen, Germany

A5

Cubic, Tetragonal, and Orthorhombic CaTiO3: Structural, Electronic and Optical Properties by First Principles Calculations

Medeiros, SK[1],Costa e Silva, J[1], Freire, VN[2], Albuquerque EL[3]
1. Universidade Federal Rural do Semi-Árido – UFERSA, Mossoró-RN, Brazil
2. Universidade Federal do Ceará- UFC, Fortaleza-CE, Brazil
3. Universidade Federal do Rio Grande do Norte – UFRN, Mossoró-RN, Brazil

A11

A comparative study of density functional methods for the optical properties of TiO2 nanowires

Ersen Mete and Hatice Unal
Department of Physics, Balıkesir University, 10145 Balıkesir, Turkey

A7

First-principles study of the structural and dynamical properties of SrRuO3

Naihua Miao, Bin Xu, Nicholas Bristowe, Matthieu Verstraete and Philippe Ghosez
Department of Physics, University of Liege, B5a, Sart Tilman, B-4000, Belgium

A5

Characterization of Hydrocarbon interaction with Carbonate and Silica Surfaces through First Principles Solid-State NMR and simulated AFM

Rochele C. A. Bevilaqua1, Vagner A. Rigo1, Caetano R. Miranda1
1.Universidade Federal do ABC – UFABC - Santo André-SP – Brazil

A6

Atomic scale insights into Ethanol oxidation on metallic nanofilms: a first principles study with van der Waals interactions

Aline O. Pereira1 and Caetano R. Miranda1
1.Universidade Federal do ABC (UFABC) – Santo André – SP – Brazil

A6

Study of 3-O-Caffeoylquinic Acid: a quantum chemical approach using electronic and vibrational spectra

Soni Mishra1, Poonam Tandon2, Pinkie J. Eravuchira3, Rasha M El-Abassy3 and Arnulf Materny3
1. Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore 560012, India 2. Department of Physics, University of Lucknow, Lucknow 226007, India 3. Chemical Physics, Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

A7

Topological defect formation and activation in carbon nanostructures

Mukul Kabir
Indian Institute of Science Education and Research, Pune – 411021, India

A1

Microscopic charge fluctuations in hexagonal boron nitride
Adela Nicolaev1,2, Claudia Rl1, Giulia Pegolotti1, Ralf Hambach1, Lucia Reining1
1 Laboratoire des Solides Irradies, UMR 7642, CNRS-CEA, Ecole Polytechnique, F-91128 Palaiseau, France and European Theoretical Spectroscopy Facility (ETSF) 2 University of Bucharest, Faculty of Physics, Materials and Devices for Electronics and Optoelectronics Research Center, P.O. Box MG-11, 077125 Magurele-Ilfov, Romania
A7

Ideal Energy-Level Alignment at the ZnO/P3HT Photovoltaic Interface
Keian Noori and Feliciano Giustino
Department of Materials, University of Oxford, Parks Road, Oxford, OX1 3PH, United Kingdom
A1

First-principles calculations of the structural and electronic properties of zinc blende B$_x$In1−$_x$N
O. D. Ojuh, 1, 2, J. O. A. Idiodi 1.
1. Physics Department, University of Benin, Benin City, Nigeria. 2. Department of Basic Sciences, Benson Idahosa University, Benin City, Nigeria
A10

The effect of ligand adsorption on the structure of metal nanoparticles
Jimena A. Olmos-Asar, Mart´ın Luduen˜a and Marcelo M. Mariscal
Departamento de Matematica y Fısica, Facultad de Cs. Quımicas. Universidad Nacional de Cordoba, Ciudad Universitaria, 5000 Cordoba. Argentina
A1

Scattering potentials of defects on Ge(001) surfaces
Tomoya Ono
Graduate School of Engineering, Osaka University, Japan
A6

Optical properties of ordered defect compounds for $CuIn_5Se_8$ and $CuIn_3Se_5$: An ab-initio study
S. Kumar1, Suman Pandey1, S. Auluck3
1. Applied Physics Department, Institute of Engineering and Technology, M. J.P. Rohilkhand University, Bareilly-243006, INDIA.
2. National Physical Laboratory, New Delhi-110012, INDIA
A7

Calculating quasiparticle energy-level alignments at molecule/semiconductor interfaces
Christopher E. Patrick, Feliciano Giustino
Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, UK
A1

Fundamental limits on transparency: first-principles calculations of absorption
H. Peelaers1, E. Kioupakis2, C.G. Van de Walle1
1. Materials Department, University of California, Santa Barbara, California 93106-5050 2. Department of Materials Science and Engineering, University of Michigan, Ann Arbor, Michigan 48109
A5

Atomic-scale insight into self-segregation and diffusion processes on a Ni/Cu bimetallic surface
Michele Rizzi1, Sara Furlan2, Maria Peressi3, Alfonso Baldereschi4
1. University of Trieste, Dept. of Physics; presently at: EPFL. Lausanne 2. University of Trieste, Dept. of Physics; presently at: SISSA, Trieste 3. University of Trieste, Dept. of Physics, IOM-CNR Democritos and INSTM 4. University of Trieste, Dept. of Physics, IOM-CNR Democritos
A6

First principle study of donor wave functions in silicon nanowires
Guido Petretto[1,2,3], Alberto Debernardi[1], Marco Fanciulli[1,2]
1. Laboratorio MDM, IMM - CNR, via C. Olivetti, 2 I-20864 Agrate Brianza (MB) Italy 2. Dipartimento di Scienza dei Materiali, Universita degli Studi di Milano- Bicocca, via Cozzi 53, I-20125 Milano, Italy
3. Present address: CEA, DEN, SRMP, F-91191 Gif-sur-Yvette, France
A1

The evaluation of perovskite phase transitions using AIDA, a materials informatics platform for materials design and discovery
Giovanni Pizzi[1], Andrea Cepellotti[1], Samed Halilov[2], Boris Kozinsky[3], Marco Fornari[4], Nicola Marzari[1]
1. Theory and Simulation of Materials, Ecole Polytechnique Fed´erale de Lausanne, Switzerland 2. Department of Materials Science and Engineering, Massachusetts Institute of Technology, USA
3. Research and Technology Center, Robert Bosch LLC, Cambridge MA, USA 4. Department of Physics, Central Michigan University, USA
A10

First-Principles Study on Carbon Emission Process at 4H-SiC(0001) Surfaces and 4H-SiC(0001)/SiO2 Interfaces
Shoichiro Saito1, Yoshitada Morikawa1, Tomoya Ono1
1. Graduate School of Engineering, Osaka University
A1

Influence of Al concentration on the opto-electronic properties of Al-doped MgO
N. Sarmadian1,R. Saniz2,D. Lamoen3 and B. Partoens 4
1-4.CMT and EMAT, Departement Fysica, Universiteit Antwerpen, Groenen-borgerlaan 171, B-2020 Antwerpen, Belgium
A7

DFT Studies on the Adsorption of Atomic Sulfur and Methanethiolate at Coinage Metal Surfaces
Porntip Seema, Jorg Behler, and Dominik Marx
Lehrstuhl fur Theoretische Chemie, Ruhr-Universitat Bochum, D-44780 Bochum, Germany
A6

CHP molecule filling the pores of the h-BN/Rh(111) nanomesh: A computational study
Jaime Gomez Dıaz[1], Ari P Seitsonen[1], Marcella Iannuzzi[1], Jurg Hutter[1]
1. Physikalisch-Chemisches Institut, University of Zurich, Winterthurerstrasse 190, CH-8057 Zurich, Switzerland
A1

Electronic structure calculations on MX2 dichalcogenide/Graphene hybrid structures.
J. A. Silva-Guillen[1], E. Cappelluti[2], R. Roldan[2], F. Guinea[2], P. Ordejon[1]
1. Centre d'Investigacio´ en Nanciencia i Nanotecnologia - CIN2 (CSIC-ICN). 08193 Barcelona, Spain 2. Instituto de Ciencias de Materiales de Madrid - ICMM (CSIC). 28049 Madrid, Spain
A1

Structural and Electronic Properties of IV Nanowires: Ab-initio Study
Anurag Srivastava, Neha Tyagi
Advance Materials Research Group, Computational Nanoscience and Technology Lab, ABV-Indian Institute of Information Technology and Management, Gwalior- 474015 (M.P.) India
A1

Size dependent electronic properties of ZnO nanowire: Ab-initio study
Anurag Srivastava, Neha Tyagi
Advance Materials Research Group, Computational Nanoscience and Technology Lab, ABV-Indian Institute of Information Technology and Management, Gwalior- 474015 (M.P.) India
A1

Optimal interface doping at La2/3Sr1/3MnO3/SrTiO3(001) heterojunctions for spintronic applications

C. Wang[1], N. Stojic[1,2], N. Binggeli[1,2]
1. Abdus Salam International Centre for Theoretical Physics, Strada Costiera 11, Trieste 34151, Italy 2. IOM-CNR Democritos, Trieste, I-34151, Italy

A3

Large-scale simulations of molecular self-assembly on epitaxial graphene on Ru (0001)

D. Stradi [1,3], C. Dıaz [1], M. Garnica [2,3], S. Barja [2,3], F. Calleja [2,3], M. Alcamı [1], N. Martın [3,4], A. L. Vazquez de Parga [2,3], R. Miranda [2,3], F. Martın [1,3]
1. Departamento de Quımica, Universidad Autonoma de Madrid, 28049, Madrid, Spain 2. Departamento de Fisica de la Materia Condensada, Universidad Autonoma de Madrid, 28049, Madrid, Spain
3. IMDEA Nanociencia, 28049, Madrid, Spain 4. Departamento de Quımica Organica, Universidad Complutense de Madrid, 28040, Madrid, Spain

A6

Heteroepitaxy of nanocrystalline Silicon Carbide on Si(111) at Room Temperature

Simone Taioli, Roberto Verucchit, Lucrezia Aversa, Marco V. Nardi, Silvio A.
Beccara, Lucia Nasi, Francesca Rossi, Giancarlo Salviati, Salvatore lannotta, and Dario AIfe
lstituto dei Materiali per I'Elettronica ed il Magnetismo, IMEM-CNR, sezione FBK di Trento, 38123 Trento, Italy
lnterdisciplinary Laboratory for Computational Science, FBK-CMM and Univ. of Trento, 38123 Trento, Italy
Department of Physics, University of Trento, Italy IIstituto Nazlonale di Fisica Nucleare, Sez. di Perugia,Italy
Dipartimento di Chimica, Universitÿ di Bologna, Italy
Department of Earth Sciences, Department of Physics and Astronomy, and London Centre for Nanotechnology, University College London, Gower Street, London, WCIE 6BT, UK
lstituto dei Materiali per I'Elettronica ed HI Magnetismo, IMEM-CNR, Parco Area delle Scienze 371A - 43124 Parma, Italy

A6

Structures and Electronic Properties of Different Orientations of C60 Encapsulated in Arm-chair Carbon Nanotubes

Savaş Berber1, Songül Üstündağ1
Gebze Instıtute of Technology, Department of Physics

A1

First-Principles Exploration of High Energy Facets of Bismuth Chalcogenide Nanocrystals

Naunidh Virk1, Oleg V. Yazyev[2] 1. Institute of Theoretical Physics, E´cole Polytechnique F´ed´erale de Lausanne
(EPFL), CH-1015 Lausanne, Switzerland.

A1

Ab initio path-integral simulations of nuclear quantum effects in hydrogen bonded ferroelectrics

Kjartan Thor Wikfeldt[1], Angelos Michaelides[2]
1. Science Institute, University of Iceland; Nordita, Stockholm; London Centre for Nanotechnology and University College London 2. London Centre for Nanotechnology and University College London

A11

Density Functional Theory (DFT) Studies of Polybromide chains in carbon nanomaterials

Abu Yayaa,B, Chris Ewelsb, Irene SUAREZ-Martinezb,C ,Serge Lefrantb, Alexandr Okotrovd, Lyubov Bulushevad, Patrick Briddone
a Dept. of Materials Science & Engineering, University of Ghana, Ghana (current address) b PMN, Institut des Materiaux Jean Rouxel, CNRS, Universite de Nantes, 44322 Nantes, France c Curtin University of Technology, Perth, Australia (current address) d Nikolaev Institute of Inorganic Chemistry SB RAS, pr. Ak. Lavrentieva 3, Novosibirsk, Russia. e Department of Electrical Engineering, Newcastle University, Newcastle-Upon-Tyne, UK

A1

Spin crossover induced by an electric bias in nanoscale devices

H. Hao. X.H. Zheng, Z. Zeng
Key Laboratory of Materials Physics, Institute of Solid State Physics,
Chinese Academy of Sciences, Hefei 230031, China

A3

Stability and kinetics of divacancy defects in bilayer graphene from first principles

Jon Zubeltzu Sese1, Emilio Artacho1,2
1. Nanogune and DIPC, Tolosa Hiribidea 76, 20018 San Sebastian, Spain 2. Department of Physics,
University of Cambridge, J. J. Thomson Avenue, Cambridge CB3 0HE, United Kingdom

A1