The Abdus Salam
International Centre for Theoretical Physics

15th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods

13 - 15 January 2011

(Miramare, Trieste, Italy)

Co-sponsored by:
International School for Advanced Studies (SISSA)
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Workshop Website:
http://agenda.ictp.it/smr.php?2220

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C O N T E N T S

P R O G R A M M E

(as of 21 December 2010)

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The Abdus Salam
International Centre for Theoretical Physics

15th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods

Organizer(s): Stefano Fabris, Lucia Reining, Ivo Souza; Local Organizer: R. Gebauer
Trieste - Italy, 13 - 15 January 2011

Venue: Leonardo da Vinci Building Main Lecture Hall

Preliminary Programme

REGISTRATION AND WELCOME (Room:Leonardo da Vinci Building Main Lecture Hall)

13 January 2011

08:00 - 08:50 (Room: Leonardo da Vinci Building, Lobby)
Registration

08:50 - 09:00 **Organizing Committee**
Introduction and opening comments

TOPOLOGICAL INSULATORS (Room:Leonardo da Vinci Building Main Lecture Hall)
Chairperson: Raffaele Resta

13 January 2011

09:00 - 09:30 **Joel Moore** / *University of California, Berkeley, USA*
Topological insulators: overview and interface/nanostructure effects

09:30 - 10:00 **David Vanderbilt** / *Rutgers State University of New Jersey, Piscataway, USA*
Orbital magnetoelectric effects and topological insulators

10:00 - 10:30 (Room: Leonardo da Vinci Building, Lobby)
--- COFFEE BREAK ---

THEORETICAL SPECTROSCOPY (Room:Leonardo da Vinci Building Main Lecture Hall)
Chairperson: Stefano Baroni

13 January 2011

10:30 - 11:00 **Claudia Ambrosch-Draxl** / *University of Leoben, Leoben, Austria*
Many-body effects in photo-emission spectra: The role of electron-phonon coupling

11:30 - 12:00 **Emmanouil Kioupakis** / *University of California, Santa Barbara, USA*
Auger recombination and absorption loss processes in nitride light emitters from first principles

12:00 - 12:30 **John Rehr** / *University of Washington, Seattle, USA*
Calculations of optical spectra from the UV-Vis to X-rays

12:30 - 14:00 (Room: Leonardo da Vinci Building Cafeteria)
--- Lunch ---

METHODOLOGICAL DEVELOPMENTS I (Room:Leonardo da Vinci Building Main Lecture Hall)
Chairperson: Erik Koch

13 January 2011

14:00 - 14:30 **Eberhard K.U. Gross** / *Max Planck Institute of Microstructure Physics, Halle, Germany*
Exact factorization of the time-dependent electron-nuclear wavefunction

14:30 - 15:00 **Evert J. Baerends** / *VU University, Amsterdam, Netherlands*
A perspective on density matrix functional theory for ground state and excited state energy surfaces

15:00 - 15:30 **Alexandre Tkatchenko** / *Fritz Haber Institut, Berlin, Germany*
Towards accurate modeling of van der Waals interactions in complex materials

15:30 - 16:00 (Room: Leonardo da Vinci Building, Lobby)
--- COFFEE BREAK ---

METHODOLOGICAL DEVELOPMENTS II (Room:Leonardo da Vinci Building Main Lecture Hall)
Chairperson: Giulia Galli

13 January 2011

16:00 - 16:30 **Giovanni Bussi** / *Istituto Nanoscienze CNR, Modena, Italy*
Stochastic thermostats in classical and ab initio molecular dynamics

16:30 - 17:00 **Ralph Gebauer** / *ICTP, Trieste, Italy*
Computational study of optical and structural properties of an organic dye sensitized solar cell

17:00 - 17:30 **Stefan Goedecker** / *University of Basel, Basel, Switzerland*
Harnessing the power of new computer hardware for electronic structure calculations with the BigDFT code

17:30 - 17:45 **Giorgio Rossi** / *Laboratorio Nazionale T.A.S.C.- CNR IOM, Trieste, Italy*
NFFA Distributed Research Infrastructure for Nanoscience: Experimental and Theory Laboratories

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

13 January 2011

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

PRESSURE AND TEMPERATURE EFFECTS (Room:Leonardo da Vinci Building Main Lecture Hall)
Chairperson: Emilio Artacho

14 January 2011

09:00 - 09:30 **Warren Pickett** / *University of California, Davis, USA*
Mott Transition in MnO and Valence Transition in Yb under Pressure: Critical Overview of an All-Electron LDA+DMFT Implementation

09:30 - 10:00 **Olle Eriksson** / *Uppsala University, Uppsala, Sweden*
Self-consistent ab-initio lattice dynamics (SCAILD); theory and numerical examples

10:00 - 10:30 **Ma Yanming** / *State Key Laboratory of Superhard Materials, Changchun, P.R. China*
Crystal structure prediction via particle swarm optimization: principles and applications

10:30 - 11:00 (Room: Leonardo da Vinci Building, Lobby)
--- COFFEE BREAK ---

MATERIALS I (Room:Leonardo da Vinci Building Main Lecture Hall)
Chairperson: Massimiliano Stengel

14 January 2011

11:00 - 11:30 **Silvia Picozzi** / *Consiglio Nazionale delle Richerche, CNR-SPIN L'Aquila, Italy*
Multiferroics: Electronic degrees of freedom at play

11:30 - 12:00 **Robert O. Jones** / *Forschungszentrum Jülich, IFF, Jülich, Germany*
Simulations of phase change materials: Order-disorder phase transitions in nanoseconds

12:00 - 14:00 (Room: Leonardo da Vinci Building Cafeteria)
--- LUNCH ---

FUNCTIONALS, ELECTRON CORRELATIONS (Room:Leonardo da Vinci Building Main Lecture Hall)
Chairperson: Nicola Marzari

14 January 2011

14:00 - 14:30 **Georg Kresse** / *Centre for Computational Materials Physics, Vienna, Austria*
Total energies from diagrammatic techniques: RPA, MP2 and coupled cluster

14:30 - 15:00 **Klaus Capelle** / *Universidade Federal do ABC, Santo André, Brazil*
Filling gaps in our understanding of gaps

15:00 - 15:30 **Neepa Maitra** / *City University of New York, USA*
Charge transfer and other challenges in TDDFT

15:30 - 16:00 (Room: Leonardo da Vinci Building, Lobby)
--- COFFEE BREAK ---

MATERIALS II (Room:Leonardo da Vinci Building Main Lecture Hall)
Chairperson: Francesco Mauri

14 January 2011

16:00 - 16:30 **Thomas Bligaard** / *Technical University of Denmark, Lyngby, Denmark*
Towards catalysis informatics

16:30 - 17:00 **Oleg Yazyev** / *University of California, Berkeley, USA*
Modeling dislocations and grain boundaries in graphene

SESSION IN HONOUR OF MATTHIAS SCHEFFLER (Room:Leonardo da Vinci Building Main Lecture Hall)
Chairperson: Richard Martin

14 January 2011

17:00 - 17:10 **Introduction of Keynote Speaker**

17:10 - 18:00 **Klaus Kern** / *Max-Planck Institut für Festkorperforschung, Stuttgart, Germany*
Keynote talk: Surfaces in and out of equilibrium

18:00 - 18:30 **Matthias Scheffler** / *Fritz Haber Institut der Max Planck Gesellschaft, Berlin, Germany*
Remarks and informal birthday session

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

14 January 2011

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

SPEEDING UP GW AND BSE (Room:Leonardo da Vinci Building Main Lecture Hall) (**Saturday**)
Chairperson: Xavier Gonze

15 January 2011

09:00 - 09:20 **Jan A. Berger** / *Ecole Polytechnique, Palaiseau, France*
Ab initio calculations of electronic excitations: collapsing spectral sums

09:20 - 09:40 **Paolo Umari** / *CNR INFM Democritos, Trieste, Italy*
GW quasi-particle spectra from occupied states only: application to DNA

09:40 - 10:00 **Feliciano Giustino** / *University of Oxford, Oxford, UK*
GW calculations for solar energy materials using the self-consistent Sternheimer equation

10:00 - 10:20 **Dario Rocca** / *University of California, Davis, USA*
Berthe-Salpeter equation without empty electronic states applied to charge-transfer excitations

10:20 - 10:35 **Discussion**

10:35 - 11:00 (Room: Leonardo da Vinci Building, Lobby)
--- COFFEE BREAK ---

THERMAL AND ELECTRONIC TRANSPORT (Room:Leonardo da Vinci Building Main Lecture Hall) (**Saturday**)
Chairperson: Jisoon Ihm

15 January 2011

11:00 - 11:30 **Takahiro Yamamoto** / *University of Tokyo, Tokyo, Japan*
Phonon transport of carbon nanotubes in ballistic, diffusive and localized regimes

11:30 - 12:00 **Stefan Kurth** / *European Theoretical Spectroscopy Facility, San Sebastian, Spain*
Dynamical Coulomb blockade and the derivative discontinuity: a not-so-steady state

12:00 - 12:30 **Duan Wenhui** / *Tsinghua University, Beijing, P.R. China*
Transport in graphene nanostructures

12:30 - 13:00 **Closing remarks**

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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)

Topological insulators: overview and interface/nanostructure effects

Joel E. Moore[1]

[1] UC Berkeley and Lawrence Berkeley National Laboratory

2D and 3D insulators can have protected edge or surface states as a result of topological properties of the bulk wavefunctions induced by spin-orbit coupling. We review the theoretical understanding of this behavior and its experimental confirmation by angle-resolved photoemission. The surface state of a 3D topological insulator such as Bi2Se3 is a reduced version of graphene with a single valley and a single spin state at each momentum. The surface states become especially important in thin films or nanowires, and we discuss electronic structure and transport aspects in these cases in the context of potential spintronic and thermoelectric applications. The surface states become gapped in the presence of time-reversal-breaking perturbations, which can be used to derive another characterization of topological insulators.

Orbital magnetoelectric effects and topological insulators

David Vanderbilt[1]

[1] Department of Physics and Astronomy, Rutgers University

The concepts of the Berry potential and Berry curvature play an important role in the theories of electric polarization, orbital magnetization, and the anomalous Hall effect. I shall briefly review these topics, and then discuss how these concepts can be applied to develop a theory of the linear orbital magnetoelectric effect in multiferroic insulators. Remarkably, there is a geometric contribution to the magnetoelectric tensor that depends on the Berry potential and curvature in a way that is more complicated than, but highly analogous to, the Berry-phase polarization expression. For example, this geometric magnetoelectric coupling theta is only well-defined modulo 2π; shifting it by a quantum corresponds to the addition of a a surface layer exhibiting an integer quantum Hall effect, just as shifting P by 2π corresponds to the occupation of an extra surface-state band. In a development that may seem unrelated, considerable excitement has surrounding the recent theoretical prediction and experimental discovery of "strong topological insulators" (STI). These are insulators that obey time-reversal (T) symmetry but which cannot be adiabatically connected to ordinary nonmagnetic insulators without a gap closure. One can show, however, that a T-symmetric insulator must have a theta of either be 0 or π; these cases correspond to ordinary insulators STI, respectively. I shall discuss the implications of these observations. This work was done in collaboration with S. Coh, A.M. Essin, A. Malashavich, J.E. Moore, I. Souza, and A.M. Turner.

Many-body effects in photo-emission spectra: The role of electron-phonon coupling

Claudia Ambrosch-Draxl,[1] *Asier Eiguren*[2]

[1] Chair of Atomistic Modelling and Design of Materials, Montanunivsersitaet Leoben, Franz-Josef-Strae 18, A-8700 Leoben, Austria
[2] Donostia International Physics Center (DIPC), Paseo Manuel de Lardizabal 4, 20018 Donostia-San Sebastin, Spain

I will highlight the impact on electron-phonon coupling (EPC) on the electronic structure, the fingerprints of which can clearly be seen in photoemission experiments. To this extent, the GW approach is employed, solving the complex Dyson equation, with the bare electronic bands as well as the Eliashberg function calculated from first-principles. It will be shown that EPC gives rise to complicated temperature-dependent band splittings in the order of the phonon frequencies. This effect can, generally, show up in arbitrary systems. It will be first illustrated for simple models, following and extending the work by Engelsberg and Schrieffer (Phys. Rev. 131, 993 (1963)). Thereafter, realistic materials such as the hydrogen-covered W(110) surface or the superconductor MgB2 will be discussed. An outlook will be given to the question whether kinks seen in photoemission data of high-temperature superconductors can be traced back to EPC.

Auger recombination and absorption loss processes in nitride light emitters from first principles

Emmanouil Kioupakis[1]

[1] Postdoctoral Researcher Materials Department, University of California Santa Barbara, CA 93106-5050, USA

Abstract: Nitride LEDs and lasers in the green to violet part of the visible spectrum have been very successful commercially, but their high-power performance is limited by large internal losses. Using first-principles calculations, we show that the efficiency reduction of nitride LEDs at high carrier densities can be attributed to indirect Auger recombination processes, mediated by electron-phonon coupling and alloy scattering. In addition, we find that internal reabsorption of light by free and acceptor-bound carriers limits the output power of nitride lasers. Our results identify the microscopic mechanisms responsible for the efficiency reduction, and suggest ways to improve the performance of nitride optoelectronic devices.

Calculations of Optical Spectra from the UV-Vis to X-rays

J. J. Rehr[1]

[1] Dept. of Physics, Univ. of Washington, Seattle, WA, 98195 USA

There has been dramatic progress in recent years in theories of optical optical and electron spectroscopies. Perhaps the most successful of these theories is based on the GW/Bethe-Salpeter Equation (GW/BSE) [1] provided strong correlations are not significant. This approach builds in several key many-body effects, which are crucial to a quantitative description over a broad spectrum. Here we discuss two complementary implementations First, a real-space approach, as in the real-space Green's function code FEFF9 [2]. For core-excitations, the GW/BSE is equivalent to an effective quasi-particle theory in the presence of a screened core-hole. Instead of approximate models, FEFF9 makes use of recentlydeveloped parameter free models, including ab initio treatments of thecore-hole interaction, inelastic losses, and Debye-Waller factors [2]. For example, the code a many-pole GW self-energy (MPSE) model to account for final state broadening and self-energy shifts. Second, we review a k-space approach, as implemented in AI2NBSE for valence spectra and OCEAN (Obtaining Core Excitation using ABINIT and NBSE) for core-spectra [3]. These hybrid codes use wavefunctions from the plane-wave pseudopotential code ABINIT together with the NIST BSE solver, and the same MPSE as above. Each of these approaches has its own advantages and disadvantages. For example, AI2NBSE and OCEAN have limited spectral ranges and require a supercell to treat aperiodic systems, while FEFF9 is applicable over a broad spectrum from the UV-x-ray energies. However, combining all of these approaches permits accurate full spectrum calculations of photon and electron spectroscopies from the UV-Vis to x-ray energies.

*Supported by DOE Grant DE-FG03-97ER45623, and facilitated by the DOE CMSN.

[1] J. J. Rehr, J. J. Kas, M. P. Prange, A. P. Sorini, Y. Takimoto, and F. Vila, Comptes Rendus Physique 10, 548 (2009).

[2] G. Onida, L. Reining, and A. Rubio, Rev. Mod. Phys. 74, 601 (2002).

[3] J. J. Rehr, F. Vila, S. D. Dalosto, E. L. Shirley and Z. H. Levine;
Phys. Rev. B 78, 205108 (2008); J. Vinson, E. L. Shirley, J. J. Rehr and J. J. Kas, UW Preprint (2010).

Exact factorization of the time-dependent electron-nuclear wavefunction

Eberhard K.U. Gross[1]

[1] Max-Planck Institut fuer Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germanyy

The coupling between electronic and nuclear motion plays an important role in a variety of phenomena. Prominent examples are superconductivity, the process of vision, and photo-synthesis. Standard approximations such as Ehrenfest dynamics, surface hopping, or nuclear wave-packet dynamics only partially capture the non-adiabatic effects. As a first step towards a full ab-initio treatment of the coupled electron-nuclear system, we deduce an exact factorization of the complete wavefunction into a purely nuclear part and a many-electron wavefunction which parametrically depends on the the nuclear configuration. We derive formally exact equations of motion for the nuclear and electronic wavefunctions [1]. These exact equations lead to a rigorous definition of time-dependent potential energy surfaces as well as time-dependent geometric phases. With the example of the hydrogen molecular ion in a laser field we demonstrate the significance of these concepts in understanding the full electron-ion dynamics. In particular, the time-dependent potential energy surfaces are shown to represent a powerful tool to analyse and interpret different (direct vs. tunneling) types of dissociation processes.

[1] Ali Abedi, Neepa T. Maitra, E.K.U. Gross, PRL 105, 123002 (2010).

A perspective on density matrix functional theory for ground state and excited state energy surfaces

Evert Jan Baerends,[1,2] *Klaas J. H. Giesbertz,*[1,2] *Oleg V. Gritsenko*[1,2]

[1] Pohang University of Science and Technology, Pohang, South-Korea.
[2] Theoretical Chemistry,Vrije Universiteit, Amsterdam, The Netherlands.

DFT owes its success primarily to affording high efficiency in the calculations, combined with quite reasonable accuracy. The high power ab initio methods scale too poorly with system size, the (semi-)empirical classical force field or heavily parametrized quantum methods still fall short of the desired accuracy. But DFT also meets with important problems. The accuracy is not guaranteed, each of the many functionals has its failure cases, and their increasing number is ominous in itself. Energies away from equilibrium geometry - energy surfaces - are problematic, both in ground state and excited states. In the calculation of response properties with TDDFT, there are grave errors when one tries to construct excited state potential energy surfaces: upon stretching of bonds the excitation energy becomes totally wrong [1] the adiabatic TDDFT method fails to describe doubly excited character [2], and fails for charge transfer transitions. All these problems stem from the difficulty that functionals working with the local density and its derivatives have in recognizing the correlation of electrons along a lengthening bond [3]. The exact position of the other nucleus, and the onset of strong correlation effects, are however manifest in orbital information: the shape and energy for occupied and virtual Kohn-Sham or natural orbitals, and the occupation numbers for the natural orbitals. Any orbital theory, being based in principle on a linear scaling number of quantities (the number of orbitals and occupation numbers) retains the promise of high efficiency. We will discuss how orbital dependent functionals can be used to describe the strong correlation in the indicated cases, both in the DFT context (with virtual orbital dependent functionals [4]) and in density matrix functional theory for ground state and excited state energy surfaces [5,6,7].

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2. K. J. H. Giesbertz, E. J. Baerends, O. V. Gritsenko, Phys. Rev. Lett. 101 (2008) 033004
3. E. J. Baerends, Phys. Rev. Lett. 87 (2001) 133004
4. M. Grning, O. V. Gritsenko and E. J. Baerends, J. Chem. Phys. 118 (2003) 7183
5. D. Rohr, K. Pernal, O. Gritsenko, E. J. Baerends, J. Chem. Phys. 129 (2008) 164105
6. K. J. H. Giesbertz, K. Pernal, O. V. Gritsenko, E. J. Baerends, J. Chem. Phys. 130 (2009) 114104
7. K. J. H. Giesbertz, O. V. Gritsenko and E. J. Baerends, Phys. Rev. Lett. 105 (2010) 013002; J. Chem. Phys. 133 (2010) 174119

Towards accurate modeling of van der Waals interactions in complex materials

A. Tkatchenko[1]

[1] Fritz Haber Institut der Max Planck Gesellschaft, Berlin, Germany

Van der Waals (vdW) forces are crucial for the structure, stability, and function of a wide variety of molecules and materials. We have recently developed a vdW-correction approach [1,2,3] that yields accuracy close to the quantum-chemical "gold standard" CCSD(T) method for inter- and intra-molecular interactions, but at a significantly reduced cost of DFT or MP2 calculations. I will discuss the theoretical underpinnings of vdW interactions in general and our method in particular, as well as its advantages/limitations compared to other available approaches. Applications for fundamental test cases will be presented: intermolecular and intramolecular interactions [1,2], organic/organic, and organic/inorganic interfaces [3-7]. The performance of our approach will be compared to both the non-local vdW-DF functional of Langreth and Lundqvist [8] and the exact-exchange plus correlation energy in the random-phase approximation (EX+cRPA). Finally, ongoing work to extend the method to describe vdW interactions in solids and adsorption problems will be discussed.

1. A. Tkatchenko and M. Scheffler, Phys. Rev. Lett. 102, 073005 (2009).
2. A. Tkatchenko, R. A. DiStasio Jr., M. Head-Gordon and M. Scheffler, J. Chem. Phys. 131, 094106 (2009).
3. N. Marom, A. Tkatchenko, M. Scheffler and L. Kronik, J. Chem. Theory Comp. 6, 81 (2010).
4. E. McNellis, J. Meyer, and K. Reuter, Phys. Rev. B 80, 205414 (2009).
5. G. Mercurio et al., Phys. Rev. Lett. 104, 036102 (2010). 7. A. Tkatchenko et al., MRS Bulletin 35, 435 (2010).
8. M. Dion et al., Phys. Rev. Lett. 92, 246401 (2004).

Stochastic thermostats in classical and ab initio molecular dynamics

Giovanni Bussi[1]

[1] Istituto Nanoscienze CNR NANO S3, Via Campi 213/A, 41100 Modena, Italy

A new molecular-dynamics algorithm for sampling the canonical distribution will be presented [1]. In this approach the velocities of all the particles are rescaled by a properly chosen random factor. Its properties will be illustrated for Lennard-Jones and water in the solid and liquid phases. Moreover, a new scheme based on colored noise Langevin equation will be presented, together with applications to Car-Parrinello molecular dynamics [2] and to the description of nuclear quantum effects [3].

1. Bussi, Donadio and Parrinello, Canonical sampling through velocity-rescaling, J. Chem. Phys. 126, 014101 (2007)
2. Ceriotti, Bussi and Parrinello, Langevin equation with colored noise for constant-temperature molecular dynamics simulations, Phys. Rev. Lett. 102, 020601 (2009)
3. Ceriotti, Bussi and Parrinello, Nuclear quantum effects in solids using a colored-noise thermostat, Phys. Rev. Lett. 103, 030603 (2009)

Computational study of optical and structural properties of an organic dye sensitized solar cell

Ralph Gebauer[1]

[1] The Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, Italy

Dye sensitized solar cells are intensely studied as possible low-cost alternatives to traditional silicon based photovoltaic devices. For further progress in this technology, a detailed understanding of the dye/semiconductor heterointerface and of the interactions of the dye molecules with the surrounding electrolyte is crucial. In this talk, I will present ab-initio molecular dynamics simulations of a dye sensitized semiconductor surface immersed in an explicit water environment. This simulation is complemented by time-dependent density functional theory computations of the optical properties of the whole system (surface + dye + solvent). This technique gives unprecedented insight into the excited states and the dynamics of the solvated system at room temperature. In particular it is shown that individual excitation spectra of instantaneous configurations are not a meaningful representation of the system's optical properties. Only averaging over many such configurations leads to a comprehensive picture that compares well with experiments. This computational technique allows the reproduction of an experimentally observed asymmetry in the absorption spectrum and provides an estimate of the effect of thermal fluctuations on the driving force for electron injection. Finally, the molecular dynamics simulations also provide a detailed picture of possible dye desorption dynamics in such systems.

Harnessing the power of new computer hardware for electronic structure calculations with the BigDFT code

Stefan Goedecker[1]

[1] Department of Physics and Astronomy,University of Basel, Basel, Switzerland

The BigDFT code is a new density functional code in the ABINIT family which uses a wavelet basis set. Being a localized and systematic basis set, wavelets combine the advantages of Gaussian and plane wave basis sets. The BigDFT code was from the beginning designed for massively parallel computer architectures. It is parallelized both with MPI and OpenMP and scales well to thousands of cores on traditional CPU's. In addition, the code is at present also ported to GPU processors using the CUDA and OpenCL programming language. This is a very promising approach which gives already at present the fastest time to solution. The Bigdft code allows to to use all common exchange correlation functionals and to perform all standard types of atomistic simulations.

Mott Transition in MnO and Valence Transition in Yb under Pressure: Critical Overview of an All-Electron LDA+DMFT Implementation

Warren Pickett[1]

[1] University of California, Davis, USA

A coupling of a dynamical mean field treatment of strong intra-atomic electronic repulsion in 3d and 4f open-shell materials with LDA (or GGA) treatment of other states has been carried out to simulate the Mott transition (insulator to metal, magnetic moment collapse, volume collapse) under pressure1, and the valence transition f14 f13 in Yb under pressure.2 The results are in fairly impressive agreement with experiment, considering how new the development of this ae LDA+DMFT approach is. Since the results are published, the predictions will be summarized only briefly. The focus of the presentation will be on the theoretical and algorithmic state-of-the-art (without getting into detail), and on the areas that need attention. This approach (and a few competitors, though they are not as widely practiced) provides the opportunity over the next decade to open up realistic simulation to the full periodic table of elements, and provide an understanding at a microscopic level of strongly correlated phenomena that have perplexed materials physicists for decades.

1 J. Kunes et al., Nature Materials 7, 198 (2008).

2. E. R. Ylvisaker et al., Phys. Rev. Lett. 103, 246401 (2009).

Self-consistent ab-initio lattice dynamics (SCAILD); theory and numerical examples

Olle Eriksson[1]

[1] Uppsala University, Uppsala, Sweden

Crystal Structure Prediction via Particle Swarm Optimization (PSO) : Principles and Applications

Yanming Ma, Yanchao Wang, Jian Lv, and Li Zhu*

State Key lab of Superhard Materials, Jilin Univ., Changchun 130012, China

We have developed a method [1] for crystal structure prediction from scratch through particle swarm optimization (PSO) algorithm. PSO technique [1] is different with the genetic algorithm and has apparently avoided the use of evolution operators (e.g., crossover and mutation). The approach is based on an efficient global minimization of free energy surfaces merging total-energy calculations via PSO technique and requires only chemical compositions for a given compound to predict stable or metastable structures at given external conditions (e.g., pressure) [1]. A particularly devised geometrical structure parameter which allows the elimination of similar structures during structure evolution was implemented to enhance the structure search efficiency. The application of designed variable unit cell size technique has greatly reduced the computational cost. Moreover, the symmetry constraint imposed in the structure generation enables the realization of diverse structures, leads to significantly reduced search space and optimization variables, and thus fastens the global structure convergence. The PSO algorithm has been successfully benchmarked in many known high pressure structures with only known information of chemical compositions for elements, binary and ternary compounds (e.g., Li, Si, C, Mg, SiO2, SiC, GaAs, TiH2, ZnO, MoB2, TiB2, MgSiO3, and CaCO3) with various chemical bonding environments, i.e., metallic, ionic, and covalent bonding [1]. The PSO algorithm has been implemented in CALYPSO code [2] and has been applied to the study on the high pressure structures of Mg [3], Li [4] and Bi2Te3. The high success rate demonstrates the reliability of this methodology and illustrates the promise of PSO as a major technique on crystal structure determination.

1. Yanchao Wang, Jian Lv, Li Zhu, and Yanming Ma, Phys. Rev. B 82, 094116 (2010).
2. Yanming Ma, Yanchao Wang, Jian Lv, and Li Zhu, http://nlshm-lab.jlu.edu.cn/ calypso.html
3. Peifang Li, Guoying Gao, Yanchao Wang, and Yanming Ma, J. Phys. Chem. C 114, 21745 (2010).
4. Jian Lv, Yanchao Wang, Li Zhu, and Yanming Ma, Phys. Rev. Lett., (in press, 2011).

Multiferroics: Electronic degrees of freedom at play

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The coexistence of long-range dipolar and magnetic orders occurs in the so-called multiferroics, one the most interesting examples of multifunctional compounds in modern materials science. In particular, electronic magnetic ferroelectrics, i.e. complex magnetic oxides in which ferroelectricity is driven by non-centrosymmetric spin- or charge- or orbital-arrangements, have recently attracted great interests. By means of density functional studies, we will focus on the existence and efficiency of different mechanisms for multiferroicity, based on the interplay between electronic and structural degrees of freedom.[1]
In closer detail, we will present cases in which a magnetically-induced electric polarization is driven by symmetric (Heisenberg-like) exchange interactions, at variance with well-known examples (such as spiral-like $TbMnO_3$), in which the polarization is induced by antisymmetric (Dzyaloshinskii-Moriya-like) exchange. Examples include orthomanganites, nickelates ($LuNiO_3$, $HoNiO_3$) or orthoferrites ($DyFeO_3$).
The second part of our presentation will be devoted to the possibility of achieving ferroelectricity induced by a non-centrosymmetric charge-order. For example, ferrimagnetic Fe_3O_4 below the Verwey transition shows an electric polarization of few $\mu C/cm^2$, induced by a charge-ordered pattern of Fe^{2+}/Fe^{3+} on the Fe B sites of the inverse spinel structure.
Finally, we will present promising avenues towards other examples where charge-ordering or spin-ordering or a combination of both spin-and-charge-ordering driven ferroelectricity can occur, in terms of novel materials, unconventional mechanisms and related efficiency.
[1] For further info, please see http://www.casti.aquila.infn.it/homepages/bismuth/index.html

Simulations of phase change materials: Order-disorder phase transitions in nanoseconds

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[2] Department of Physics, Tampere University of Technology, FI-33101 Tampere, Finland
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Phase change materials are the basis of many familiar memory devices (including DVD-RW, DVD-RAM, and Blu-ray Disc) and function because of an extremely rapid (no more than tens of nanoseconds) transformation between amorphous and crystalline phases with quite distinct optical properties and resistivity. Relatively few families of alloys satisfy the requirements of optical contrast and rapid phase transitions, and these usually have several components (e.g. Ge/Sb/Te or "GST" alloys, Ag/In/Sb/Te or "AIST" alloys). An understanding of the phase change process requires, of course, a detailed knowledge of the structures involved, which is very difficult to obtain in disordered phases of such alloys. We have performed "Car-Parrinello" type simulations of a range of such alloys, in order to characterize the amorphous phases involved. We have simulated hundreds of atoms over a time scales of hundreds of picoseconds in GeTe, Ge2Sb2Te5 (DVD-RAM) [1], Ge8Sb2Te11 (Blu-ray Disc) [2], and an AIST alloy near the Sb/Te eutectic (70:30, DVD-RW) [3]. These calculations have enabled us to identify structural patterns and to propose mechanisms for the phase transitions.

1. J. Akola and R. O. Jones, Phys. Rev. B 76, 235201 (2007); Phys. Rev. Lett. 100, 205502 (2008); J. Akola, R. O. Jones et al., Phys. Rev. B 80, 020201 (R) (2009)
2. J. Akola and R. O. Jones, Phys. Rev. B 79, 134118 (2009)
3. J. Akola and R. O. Jones, Appl. Phys. Lett. 94, 251905 (2009); T. Matsunaga et al., Nature Mater. (in press)

Total energies from diagrammatic techniques: RPA, MP2, and coupled cluster

Georg Kresse[1]

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The simplest approach to calculate total energies from diagrammatic techniques is the random phase approximation (RPA) first suggested and applied by Nozieres and Pines. With the tremendous improvements in computer performance and using efficient implementations, we are now able to apply the RPA to fairly large systems. In this talk, I present a survey of our recent results, covering lattice constants, bulk moduli, and atomisation energies of prototypical solids[1-2]. The results are generally significantly improved over conventional density functional theory calculations. Specifically, we demonstrate that predicted equilibrium volumes of alkali and alkali earth metals, transition metals and noble metals are within 1-2 percent of experiment. Setting out from this observation we apply the method to more challenging prob- lems, such as surface energies, adsorption energies of small molecules on surfaces [3], and van der Waals bonded systems (graphene) [4]. The results suggest that the RPA outperforms all available density functionals, accounting equally well for van der Waals bonding, ionic, covalent, and metallic bonding. However, a slight tendency towards underbinding is observed, making accurate predictions (chemical accuracy) not yet possible. Possible solutions to this problem, such as second order perturpation theory (MP2) and coupled cluster methods, are briefly discussed.

1. J. Harl and G. Kresse, Phys. Rev. Lett. 103, 056401-14 (2009).
2. J. Harl, L. Schimka, and G. Kresse, Phys. Rev. B 81, 115126-118 (2010).
3. L. Schimka, J. Harl, A. Stroppa, A. Gruneis, M. Marsman, F. Mittendorfer, and G. Kresse, Nature Materials 9, 741744 (2010).
4. S. Leb'egue, J. Harl, Tim Gould, J. G. A ngya n, G. Kresse, and J. F. Dobson, Phys. Rev. Lett. 105, 196401-14 (2010).

Filling gaps in our understanding of gaps

Klaus Capelle[1]

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While the presence or absence of a gap is a fundamental property of materials, our capability of reliably calculating different types of gaps within density-functional theory is still limited by deficiencies of the local-density approximation and its improvements, as well as by conceptual difficulties in defining various types of gaps. In this talk I present results addressing different aspects of this problem: (i) a local-density-type functional for a model Hamiltonian that reproduces the exact Mott gap; (ii) a numerical investigation of the role of self-interaction corrections in predicting band gaps; (iii) a simple approximation permitting to estimate derivative discontinuities of finite systems; (iv) an extension of this work from charge (Mott or band) gaps and charge discontinuities to spin gaps and spin discontinuities.

Total energies from diagrammatic techniques: RPA, MP2, and coupled cluster

Georg Kresse[1]

[1] Faculty of Physics and Center for Computational Materials Science, University Vienna, A-1090 Vienna, Austria

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2. J. Harl, L. Schimka, and G. Kresse, Phys. Rev. B 81, 115126-118 (2010).
3. L. Schimka, J. Harl, A. Stroppa, A. Gruneis, M. Marsman, F. Mittendorfer, and G. Kresse, Nature Materials 9, 741744 (2010).
4. S. Leb'egue, J. Harl, Tim Gould, J. G. A ngya n, G. Kresse, and J. F. Dobson, Phys. Rev. Lett. 105, 196401-14 (2010).

Charge-transfer and other challenges in TDDFT

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TDDFT has achieved an unprecedented balance between efficiency and accuracy for calculations of optical spectra of a wide variety of systems. However severe challenges lie in several areas, including long-range charge-transfer excitations, conical intersections, double excitations – and these are important to resolve for many applications, such as photo-induced coupled electron-nuclear dynamics, solar-cell design. We discuss some recent developments, in particular a semiclassical approach to electron correlation in density-matrix dynamics.

Towards catalysis informatics

Thomas Bligaard[1]

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Modeling dislocations and grain boundaries in graphene

Oleg Yazyev[1]

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Topological defects in graphene, dislocations and grain boundaries, are still not well understood despites the considerable number of experimental observations. In my talk, I will describe computational techniques for atomistic modeling of topological defects in materials. I will then focus on graphene by introducing a general approach for constructing dislocations characterized by arbitrary Burgers vectors as well as grain boundaries, covering the whole range of possible misorientation angles. An ab initio investigation of thermodynamic, electronic and transport properties of grain boundaries in polycrystalline graphene reveals energetically favorable large-angle symmetric configurations, strong tendency towards out-of-plane deformation in the small-angle regimes, pronounced effects on the electronic structure, and two distinct behaviors in the electronic transport either perfect reflection or high transparency for low-energy charge carriers depending on the grain boundary structure. These results show that dislocations and grain boundaries are important intrinsic defects in graphene which may be used for engineering graphene-based functional devices.

1. O. V. Yazyev and S. G. Louie, Phys. Rev. B 81, 195420 (2010).
2. O. V. Yazyev and S. G. Louie, Nature Mater. 9, 806 (2010).
Work done in collaboration with Steven G. Louie

Keynote talk

Surfaces in and out of equilibrium

Klaus Kern[1]

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Ab initio calculations of electronic excitations: Collapsing spectral sums

Arjan Berger[1]

[1] Laboratoire des Solides Irradis, Ecole Polytechnique, Palaiseau, France

We present a method for the evaluation of electronic excitations of advanced materials by reformulating spectral sum-over-states expressions such that only occupied states appear. All empty states are accounted for by one effective energy. Thus we keep the simplicity and precision of the sum-over-states approach while speeding up calculations by more than an order of magnitude. We demonstrate the power of this effective-energy technique (EET) by applying it to the GW method, where a huge summation over empty states appears twice (screening and self-energy). We show the precision of the EET for bulk silicon and argon. We then use it to determine the band structure and optical spectrum of the technologically important oxide SnO2. We will also show how the EET can be used to develop exchange-correlation kernels for time-dependent density-functional theory that are both accurate and computationally efficient.

GW quasi-particle spectra from occupied states only: application to DNA

Paolo Umari[1]

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I will illustrate our recently introduced method [1,2] which allows for the calculation of quasi-particle spectra in the GW approximation in large systems, yet avoiding any explicit reference to empty one-electron states. This is achieved first by introducing an optimal basis set for the polarizability operator, then by expressing the irreducible polarizability operator and the self-energy operator through a set of linear response equations, which are solved using a Lanczos-chain algorithm. After validating the approach addressing the isolated benzene molecule and bulk silicon, I will illustrate its capabilities with some examples: the calculation of the photoemission spectra of porphyrin derivatives and their comparison with experimental synchrotron data, and the calculation of the electronic densities of states of some disordered materials, namely silica and amorphous silicon nitride. Finally, I will show how, using high-performance computing facilities, we could calculate GW spectra of large single strand DNA models.

1. P. Umari, G. Stenuit, S. Baroni, Phys. Rev. B , 79, 201104R (2009).
2. P. Umari, G. Stenuit, S. Baroni, Phys. Rev. B, 81, 115104 (2010).

GW calculations for solar energy materials using the self-consistent Sternheimer equation

Feliciano Giustino[1]

[1] Department of Materials, University of Oxford, Oxford OX1 3PH, United Kingdom

In excitonic solar cells the photocurrent is generated by the dissociation of excitons at the donor/acceptor interface. As a consequence of this mechanism, the open circuit voltage of the cell is determined by the energy offset between the conduction band bottom of the semiconductor and the highest occupied molecular orbital of the dye or polymer. The accurate knowledge of the interfacial band alignment is therefore crucial for the design and optimization of excitonic solar cells. A recent work on semiconductor/oxide interfaces has established the predictive power of the GW method in the band alignment problem.1 However this method relies on the calculation of a large number of unoccupied electronic states2 and is limited to small systems containing at most 50-100 atoms. In order to circumvent this difficulty we introduced an alternative approach to GW calculations based on the self-consistent Sternheimer equation.3 In this method the screened Coulomb interaction is evaluated by solving self-consistent linear-response equations as in density-functional perturbation theory, and the Greens functions is obtained by directly solving inhomogenous linear systems. In this talk I will first provide an overview of our activity in the area of excitonic solar cells. Then I will discuss the Sternheimer-GW method and present a proof-of-concept calculation for bulk silicon within the empirical pseudopotential method. Finally I will illustrate our ongoing work on realizing full-scale implementations of the method in both a plane waves and a localized orbital software packages.

* Work done in collaboration with S. G. Louie, M. L. Cohen, C. Patrick, K. Noori.

1. R. Shaltaf, G.-M. Rignanese, X. Gonze, F. Giustino, and A. Pasquarello, Phys. Rev. Lett. 100, 186401 (2008).

2. M. Hybertsen and S. G. Louie, Phys. Rev. B 34, 5390 (1986).

3. F. Giustino, M. L. Cohen, and S. G. Louie, Phys. Rev. B 81, 115105 (2010).

Bethe-Salpeter equation without empty electronic states applied to charge-transfer excitations*

Dario Rocca[1]

[1] Department of Chemistry, University of California, Davis, USA

We present an approach to compute optical absorption spectra of molecules and nanostructures from first principles, which is suitable for the study of large systems and gives access to spectra within a wide energy range. In this approach, the quantum Liouville equation is solved iteratively within first order perturbation theory, with a Hamiltonian containing a static self-energy operator [1]. This is equivalent to solving the Bethe-Salpeter equation. Explicit calculations of single particle excited states and inversion of dielectric matrices are avoided using techniques based on Density Functional Perturbation Theory [1,2]. The calculation and inclusion of GW quasi-particle corrections within this framework are discussed. The efficiency and accuracy of the new approach are demonstrated by computing optical spectra of nanostructures and charge transfer excitations.

1. D. Rocca, D. Lu and G. Galli, J. Chem. Phys. 133, 164109 (2010).
2. H. Wilson, F. Gygi and G. Galli, Phys. Rev. B , 78, 113303, 2008; H. Wilson, D. Lu, F. Gygi and G. Galli, Phys. Rev. B, 79, 245106,2009.
Work in collaboration with Yuan Ping, Deyu Lu, Huy-Viet Nguyen and Giulia Galli.

Phonon transport of carbon nanotubes in ballistic, diffusive, and localized regimes

Takahiro Yamamoto[1], *Kenji Sasaoka* [2], *Sathoshi Watanabe*[1]

[1] Department of Materials Engineering, The University of Tokyo, Japan
[2] Center for Computational Sciences, University of Tsukuba, Japan

Great attention has been paid to single-walled carbon nanotubes (SWNTs) as potential candidates for heat removal materials because of their extremely high thermal conductivity. Besides its practical importance in heat-device applications, the phonon transport in SWNTs is the subject of academic interest because it exhibits various interesting phenomena originating from the coherency of phonons in quasi-one-dimensional systems [1]. In this talk, we present simulation results on the coherent phonon transport in SWNTs obtained using the nonequilibrium Greens function (NEGF) method, such as the quantization of thermal conductance [2] and the phonon scattering by defects [3]. In particular, we discuss the case of disordered SWNTs with 13C isotopes. In contrast to classical molecular dynamics and semi-classical Boltzmann equation, the NEGF method enable us to perform fully quantum-mechanical simulations of the coherent phonon transport in an SWNT. We found that the phonon transport in the isotope-disordered SWNTs is classified into three regimes depending on the phonon frequency : the low- ballistic, the mid- diffusive, and the high- localized regimes. In the ballistic regime, the SWNTs exhibit the quantization of thermal conductance even in the presence of 13C isotopes. In the diffusive regime, the SWNTs show the universal transmission fluctuation of the order of unity regardless of the number of phonon channels. More details will be discussed in the presentation.

1. T. Yamamoto, K. Watanabe, E.R. Hernandez, Carbon Nanotubes: Advanced Top- ics in the Synthesis, Structure, Properties and Applications (Springer-Verlag, Berlin, Heidelberg 2008) pp.155-182.
2. T. Yamamoto, S. Watanabe, K. Watanabe, Phys. Rev. Lett. 92, 075502 (2004).
3. T. Yamamoto and K. Watanabe, Phys. Rev. Lett. 96, 255503 (2006).

Dynamical Coulomb blockade and the derivative discontinuity: a not-so-steady state

Stefan Kurth[1]

[1] European Theoretical Spectroscopy Facility, San Sebastian, Spain

In the description of electron transport using time-dependent density functional theory, the discontinuity of the exchange-correlation potential is shown to be intimately related to Coulomb blockade. Moreover, the discontinuity can have a profound effect on the time evolution of an interacting nanostructure attached to biased leads: instead of reaching a steady state long after the bias switch-on, the system evolves towards a dynamical state of correlation-induced density and current oscillations. We thus establish a dynamical picture of Coulomb blockade as a periodic sequence of charging and discharging of the nanostructure.

Transport in graphene nanostructures

Wenhui Duan[1]

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In this talk, I will discuss intrinsic transport properties of perfect and edge-defected zigzag graphene nanoribbons (ZGNRs) based on the first principles calculations. It is found that although all perfect ZGNRs have similar metallic band structure, they show distinctly different transport behaviors under bias voltages, depending on whether they are mirror symmetric with respect to the midplane between two edges, which originates from symmetry-dependent coupling between the conducting subbands around the Fermi level. Furthermore, the migration and recombination of edge defects (carbon adatom and/or vacancy) and their influence on electrical conductance are demonstrated for ZGNRs. Spontaneous formation of pentagon-heptagon-ring defect structure is observed, which can suppresses the conductance of ZGNRs drastically.

POSTER SESSION 1

THURSDAY 13 JANUARY 2011

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

http://agenda.ictp.it/smr.php?2220

The Abdus Salam
International Centre for Theoretical Physics

POSTER SESSION I

THURSDAY 13 JANUARY 2011

In alphabetical order of presenting author (underlined)

Beyond DFT: Taking into account charging energy and semiclassic electron-phonon coupling
Enrique Abad 1, James P. Lewis 2, Jose Ortega1 Fernando Flores 1
1.Departmento de Fısica Teorica de la Materia Condensada, Universidad Autonoma de Madrid, 28049 Madrid, Spain (email: enrique.abad@uam.es) 2. Department of Physics, West Virginia University, Morgantown, WV, USA
D1 T1 1

Ultrasoft pseudopotentials and projector augmented-wave data-sets: application to diatomic molecules
Alwaleed Ahmed Adllan 1 and Andrea Dal Corso 2
1. Al-neelain University Gamhuria Street, Khartoum, (Sudan) 2. SISSA, Via Bonomea 265, 34136 Trieste (Italy) and IOM-DEMOCRITOS Trieste
D1 T11 2

Fully self-consistent LDA+DMFT Calculations: A plane wave and projector augmented wave implementation and application to the study of Cerium compounds.
Bernard Amadon,
CEA, DAM, DIF, F 91297 Arpajon, France
D1 T3 3

First-principles study (GW+PAW) on new oxynitride phosphors for white LED
B. Bertrand 1,2, M. Mikami 3, M. Stankovski 1, X. Gonze 1
1. European theoretical spectroscopy facility (ETSF), Universite Catholique de Louvain, Louvain-la-Neuve, Belgium 2. CERDECAM, Institut Suprieur Industriel ECAM, Bruxelles, Belgium 3. Mitsubishi Chemical Group Science and Technology Research Center, Inc., Yokohama, Japan
D1 T3 4

Regarding the Structural Phase Transitions and sp-d Hybridization in Cubic Calcium
N. K. Bhatt 1*, B. Y. Thakore 1, P. R. Vyas 2, and A. R. Jani 1
1Department of Physics, Sardar Patel University, Vallabh Vidyanagar, 388 120, Gujarat, India
2Department of Physics, School of Sciences, Gujarat University, Ahmedabad, 380 009, Gujarat, India
D1 T3 5

Local Density Approximation plus Gutzwiller Method, a Siesta implementation
Giovanni Borghi
International School for advanced studies (SISSA), via Beirut 2-4, 34151 Trieste, Italy
D1 T4 6

Energetics and metastability of the silicon vacancy in cubic SiC
Fabien Bruneval
Centre d'Etudes Nucléaire de Saclay, 91191 Gif-sur-Yvette, France
D1 T3 7

Influence of biaxial strain on spinodal decomposition in magnetic semiconductor alloys
C. Caetano1, L. K. Teles2, M. Marques2, and L. G. Ferreira3
1. Universidade Federal da Fronteira Sul, Realeza, PR, Brazil 2. Instituto Tecnológico de Aeronáutica, São José dos Campos, SP, Brazil 3. Universidade de São Paulo, São Paulo, SP, Brazil
D1 A3 8

Atomic and electronic structure of Co2CrAl/NaNbO3/Co2CrAl magnetic tunnel junctions
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D1 A3 9

Solvation and thermal effects on the optical properties of natural dyes: a case study on the flavylium cyanin
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D1 T2 10

Long-wavelength properties of metallic systems studied by ab initio methods
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D1 T11 11

Dynamical response function in Sodium and Aluminum from Time-Dependent Density-Functional Theory
Marco Cazzaniga 1,2, Hans-Christian Weissker 1,3,4, Simo Huotari 5, Tuomas Pylkkanen 5,6, Giulio Monaco 5, Giovanni Onida 1,2, and Lucia Reining 1,3
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D1 T2 12

First principles EPR spectra of transition metal complexes
Davide Ceresoli and Nicola Marzari
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D1 T9 13

The projector augmented–wave method: application to relativistic spin–density functional theory
Andrea Dal Corso1,2
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D1 A3 14

Analysis of thermodynamic, thermoelectric and magnetic properties of FeSb2 in the framework of density functional theory

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D1 A3 15

Ab-initio investigation of lattice dynamics in substitutional disordered alloys

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D1 T11 16

Magnetism & magnetic anisotropies of small structures containing 5d atoms

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Centro de Investigación en Nanomateriales y Nanotecnología, CSIC and Universidad de Oviedo, 33011 Oviedo, Spain

D1 A3 17

Electronic response in Koopmans corrected functionals: polarizabilities and hyperpolarizabilities of linear chains

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D1 T1 18

First-principles study of the magnetic phase diagram of LaOx−1FxFeAs

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Electronic circular dichroism for Guanine-Cytosine base pairs in Watson-Crick and Hoogsteen configuration

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D1 T2 20

Many Body Perturbation Theory simulations of the electronic properties of large DNA models.

L. Giacomazzi1, P. Umari2, A.V. Vargiu,3 L. Martin-Samos 2, A. Magistrato 2, C. Cavazzoni 4,and S. Baroni 1,2
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D1 T3 21

The interactions of nitrogen dioxide with graphene and with Rh clusters stabilized by graphene

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D1 A1 22

Role of the Pressure in the Elastic Properties of Ce

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D1 T1 23

Local Field Effects in Silicon Nanocrystals

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D1 A7 24

Exchange an Correlation effects in photoemission spectroscopy: from semiconductors to transition metal oxides

Matteo Guzzo 1,2, Matteo Gatti 2,3, Francesco Sottile 1,2, Pina Romaniello 1,2, Fausto Sirotti 4, John Rehr 1,5, Lucia Reining 1,2
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D1 T3 25

Elasticity and Conductance interplay in model molecules

Prokop Hapala 1, Jin He 2,Pavel Jelínek 1, Stuart Lindsay 2
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D1 A1 26

Discontinuities of the Exchange-Correlation Kernel and Charge-Transfer Excitations in TDDFT

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Formalism for GW calculations without empty states in a localized basis

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Ab initio investigation of topological insulators

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Linear Response TDDFT in CASTEP: An HPC Implementation
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Total Energy Formalism for Charged Nanocapacitors: Orbital Partition Approach
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Electron-electron interactions in superconducting Lithium under pressure
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Resolving Controversies on the Multiple Conductance Peaks in Single- Molecule Junction Experiments by Multiscale Simulations
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Expanded radialenes carbon nanotubes: electronic and elastic properties
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Determination of NMR chemical shifts for cholesterol crystals from first-principles
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Pressure induced unified study of strongly correlated ErSb
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Direct calculation of the one particle Green's function: an alternative to the self-energy
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Electronic correlations at the α-γ structural phase transition in paramagnetic iron
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High-pressure Raman spectra of TiO2
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Magnetism in FeMn Nanostructures
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Study of the relaxation of the Aluminum cluster in the self-compressed inhomogeneous stabilized jellium model
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RVB states in graphene and other carbon compounds
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Spin and valley susceptibility in wide AlAs quantum wells
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A self-consistent, first-principles method for complex disordered materials
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MICROMAGNETIC SIMULATIONS OF FIELD INDUCED DOMAIN WALL MOTION IN Fe20Ni80/Cu/Co SPIN VALVE
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First-principles Study of P3HT/ZnO Hybrid Organic-Inorganic Photovoltaic Interface
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p Magnetism in CaC: First principle study
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Stability of domain boundaries on the Ge-covered 5×5-reconstructed Si(111) surface
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First-principles study of O1s core-level shifts at dye-sensitised solar cell interfaces
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Nonlinear Elasticity of Graphene and Other Hexagonal Carbon Allotropes
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Ab-initio calculations of absorption spectra of nanowires by solving the Bethe-Salpeter Equation
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Dispersion interactions in room-temperature ionic liquids: Results from a non-empirical density functional
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Edge effects in graphene nanoislands on Co(0001)
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Surface-induced magnetism in C-doped SnO2: First-principles study
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Monte Carlo modeling of structural properties in compressed 2D Wigner crystals
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Surface-induced atomic and electronic properties of unpassivated GaAs Nanowires
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Electronic properties of crystal and amorphous phases of SiO2: disorder effects within and beyond Density Functional Theory
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DFT and Beyond - Climbing Jacob's Ladder
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Polynitrogen confined to C60 Cage: A novel energetic Material
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A unified pseudopotential approach to superconducting state parameters of Mg, B and MgB2
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Electronic structure of hydrogenated diamond surfaces: The role of temperature on surface reconstruction
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The nonempirical calculations of the lattice dynamics of the oxyfluoride Rb2KTiOF5
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Pseudo-electromagnetism in graphene
Young-Woo Son
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PAW method in localized-basis-set SIESTA code: first stage of development
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A simulated reflectivity experiment: theoretical optical spectrum of strained-lattice bulk SrTiO3
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Ab initio study of electronic properties of bismuth
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Numerical simulation of four-probe resistance measurements of nanoscale materials
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Characterization of point defects in UO2 by positron annihilation spectroscopy: a first-principles study
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Electron-phonon coupling in semiconducting nanostructures
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The absorption of diamondoids from time-dependent density functional calculations
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Electrical, Optical and magnetic properties of cobalt doped titanium dioxide Thin films made by Spray Pyrolysis
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Ab initio prediction of giant magnetoelectric effects driven by structural softness
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A DFT/TDDFT study of di-zinc pyrazinoporphyrazine-phthalocyanine complexes with different peripheral substituents as potential sensitizers in a DSC
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A theoretical study of the effect of the bridge (=CH-, =N-, -O-, -S-) connecting di-Zinc pyrazinoporphyrazine-phthalocyanine complexes
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Optical properties and aromaticity of meso substituted porphyrins
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The role of van der Waals forces in semiconductor solids
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The full abstract can be found on the Workshop's website:

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The Abdus Salam
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POSTER SESSION II

FRIDAY 14 JANUARY 2011

In alphabetical order of presenting author (underlined)

Optical Properties of α−Se Revealed by ab initio Calculations
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Electronic structure, magnetic ordering and structural instabilities of cubic perovskites based on nitrides and fluorides: A comparative first-principles study
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Magnetostructural dynamics of a Rieske-type [2Fe-2S] protein
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Adsorption of rare-gas atoms and water on graphite and graphene by van der Waals-corrected Density Functional Theory
A. Ambrosetti, F. Ancilotto, F. Toigo and P. L. Silvestrelli
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First-principles study of the Sr3Ru2O7 electronic structure and its effective tight binding description
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Optoelectronic properties of Al:ZnO: critical dosage for an optimal transparent conductive oxide.
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Thermal transport in nanomaterials from first-principles
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Charge Localization Dynamics Induced by Oxygen Vacancies on the TiO2(110) Surface
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Oxidation at the Si(100) surface studied by theoretical high-resolution EELS
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A comparative study of Sin and Snn (n = 1-6) clusters On MgO Surface: An ab-initio method based study
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Modelling yttrium aluminosilicate glass for radiotherapy
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Insights into point defects in silicon from large-scale DFT calculations and maximally-localized Wannier functions
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Structural, thermodynamic and electronic analysis of Zn-Al-Cl LDH exchanged by F−, Br−, OH−, NO−3 , PO−3 and CO2−: A ab initio study. 3
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First-principles investigation of new phases of BiFeO3 and of the BiFeO3-BiCoO3 solid solution
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Mechanochemistry, Metadynamics, QM/MM
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Enhancement of catalytic activity on bimetallic Ni/Cu(110): a first principles study

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Molecular Dynamic Simulation Studies of the Collision of a Non-rotranslating Diatomic H2 / D2 (v=0,j=0) Molecule with Copper Atomic Cluster (cu13)

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Novel Structures, Superconductivity and Anharmonicity of Calcium Under Pressure from ab initio Calculations

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Direct comparison between two γ-Al2O3 models by DFT calculations

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Crystallization on heating of α-cyclodextrin solutions

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Growth and electronic properties of low-dimensional Fe/Au(111) structures

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Early stages of Pd adsorption on Au(111)
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Ab initio investigation of ZrO2-CeO2 interface properties
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Ab-initio study of the structural and electronic properties of InAs/GaAs radial heterostructures
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First principle study of hydroxyl functional groups on pristine defected graphene and graphene epoxide
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Catalytic activity of gold nanoclusters supported by cerium oxide: interplay between cluster morphology, size and adsorbate stability revealed by DFT+U calculations
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First-principles study of Bi1−xLaxFeO3 multiferroic solid solutions
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Incorporation of iron on the clean and gallium-bilayer GaN(0001) surface
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First-principle approach to the temperature dependence of electronic energies.
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First Principles Study of Cr Doping on Structural Properties of LiMn2O4
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Melting of Hydrogen at High Pressures from Ab-initio Molecular Dynamics Coexistence Simulations
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Pressure-induced transitions from sp2 to sp3 structures in BN
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Ab-initio Models of Disordered Phases of Ice
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Angular dependence of interaction energy components in ammonia – hydrogen halide complexes. Application of Symmetry-Adapted Perturbation Theory
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First-principle calculations of vacancy-hydrogen interactions in iron: V_nH_m systems (n = 1, 3; m = 1, 6)
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BRAGG-WILLIAMS MODEL OF ORDERED B2, L12 and L10 TYPE BINARY INTERMETALLIC COMPOUNDS CONTAINING POINT DEFECTS

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Theoretical investigation of elastic properties of hexagonal boron nitride membranes (h-BN)

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Superlattices based on graphene and graphane. Theoretical investigation of electronic properties

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First-principle calculations of magneto-optical properties of rare earth RAl2 (R = Ce and Pr) compounds

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The energetics induced by interstitial C in Ti-Al-Nb alloys

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Ab initio study of the crystallization kinetics of phase-change materials

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Catalytic Water Splitting for Hydrogen Production: A First-Principles Study of a Ru Complex in Solution

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Comment to "Imaging the atomic orbitals of carbon atomic chains with field-emission electron microscopy"

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Long-range ordered surface alloy of bulk-immiscible components stabilized by magnetism: Fe-Au/Ru(0001)

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Stacking and Registry Effects in Layered Materials: The Case Of Hexagonal Boron Nitride

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Stability of Methane with respect to dissociation and other C-H stoichiometries under pressure

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XPS of amorphous CdTeOx: validation of a structural model

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First principles study of the $LiNH_2/Li_2NH$ transformation

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First principles studies of molecular confinement and degradation in cement

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Promotion of Ethylene Epoxidation Selectivity by Subsurface Oxygen in Ag-Cu Alloy Catalysts
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Structure and Chemical Reactivity of Small Pt Clusters on a Carbon Nanotube: A First-principles Study
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A quantum chemical study on Polythiophenes derivatives as donor materials in bulk-heterojunction polymer solar cells
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Symmetry-Adapted Perturbation Theory study of intermolecular interaction energy between organic molecules with three- and four- membered rings.
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A first principles study of hydrogen and ethanol adsorption on Pd based metallic nanofilms
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Lithium storage and diffusion on inorganic nanotubes from first principles
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Ab-initio modelling of Ru-based homogeneous catalysts for water oxidation
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Ab-initio parameterisation of inter-atomic force fields for the description of solid-solid and liquid-solid interfaces
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Azobenzenes Self Assembled Monolayers
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Ab initio modelling of interfaces: TiO2 grown on A12O3 as a prototype
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Theoretical investigations on the TMG (trimetylogallium) adsorption and the TMG diffusion on the GaN (gallium nitride) surface.
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Structural and electronic properties of GaN surfaces (0001) and (000-1) due to the presence of molecules nearby of the slab face obtained from DFT
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The calculation of experimental spectra using linear-scaling densityfunctional theory
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Imaging and characterization of activated CO2 species on Ni(110)
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Accurate ab initio parametrised atomistic force fields for ionic materials: application to alumina
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Computational studies of the h-BN nanomesh on Rh(111) surface
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Ab-initio investigations of platinum oxides
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Titania-silica interfaces: a combined classical and DFT study.
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Electronic properties of intermetallic Ti3Al
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Raman spectra of amorphous phase change materials from first principles
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H2CO3 forms via HCO−3 in water
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Nanoscale engineering of surface stress
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A Theoretical Investigation of Structural, Mechanical and Electronic Properties of some late Transition-Metal Nitrides
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Vibrational Spectroscopy and Density Functional Theory of Intermolecular Hydrogen Bonding in 2-Thiohydantoins.
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Surface Precursors and Reaction Mechanisms for the Thermal Reduction of Graphene Basal Surfaces Oxidized by Atomic Oxygen
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Atomistic Simulation of Co-doped α-Alumina Interfaces
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First principles non-equilibrium Green's function study of Ta2O5 atomic switch
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Mechanical properties of icosahedral boron carbide explained from first principles
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DFT+U study of oxygen migration processes in nickle doped ceria
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p-type doping and codoping of ZnO based on nitrogen is ineffective: an ab initio clue
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