The Abdus Salam
International Centre
for Theoretical Physics

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

15 - 17 January 2015
Trieste - Italy
Cosponsor(s) CECAM, Consorzio per la Fisica di Trieste, Psi-k and SISSA

POSTER SESSION I

THURSDAY, 15 JANUARY 2015

In alphabetical order of presenting author (underlined)

Study of Electronic Properties of BC2N Nanotubes

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

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Electrostatics of solvated systems in periodic boundary conditions

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Structural and electronic properties of Polyacetylene chains through Variational Monte Carlo

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Solvation effects on the color optical properties of anthocyanin natural dyes

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Solution of the many-body problem in one point

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

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

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

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

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Light-induced field enhancement in polyacenes

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

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

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Surface-assisted formation of grapheme nanoribbons on Au surfaces

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Electron energy loss anisotropies in MAX phases: Ti2AlC

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Phonon Hydrodynamics in Two-Dimensional Materials

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

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

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

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

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DFT study of the reactivity of CO2 in molten alkali carbonates

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

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First-principles study of Radical Organic Electrodes

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On the interpretability of molecular orbitals from organic semiconductors

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Transport Properties of Iron-Porphyrin / Graphene Junction

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

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

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

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Thermoelectric properties of n-doped Silicon from first-principles

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A generalized Poisson solver for complex electrostatic environments

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Anchoring and Bending of Pentacene on Aluminum (001)

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Enhanced Atom Mobility on the Surface of a Metastable Film

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

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Resonant Lifetime of Core-Excited Organic Adsorbates from First Principles

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A general method for functional optimization

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Subsystem Density Functional Theory for Periodic Systems

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Effects of anion doping on oxide-metal interface: a DFT study of MgO/Mo

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Unravelling the origin of the E'α and Ge(2) centers

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Local Reduced Density Matrix Functional Theory

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Magnetic Anisotropy Energy in Narrow Silicene Nanoribbons

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Speeding up linear-response DFT calculations with optimally reduced plane-wave basis sets

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Ferromagnetic iron as a topological metal

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High performance electronic structure engineering with hybrid DFT and GW

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

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

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Electronic and Optic Properties of Corrugated Quantum Wells

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Valence Band Structure of Square Quantum Well Under Stress

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

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

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

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Thermoelectricity: Coupling transport equations and *ab initio* calculation

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Interplay between defects and stacking at the SiC/SiO2 interface

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A General Purpose Massively Parallel *Ab Initio* Molecular Dynamics Implementation With A Linear Scaling Exact Exchange Algorithm

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First-Principles Study Of Oxide Superlattices

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

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Metal-Insulator Transition and Lattice Instability of Paramagnetic V2O3

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Study of Electronic Properties of BC_2N Nanotubes

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Hexagonal BC_2N is the most stable stoichiometry in a group of compound $B_xC_yN_z$ hybrid nanostructures. It can be produced as a graphite-like layered structure consisting stacked hexagonal sheets with an intralayar lattice constant and interlayer distance very similar to the values for graphite. It is believed that the stabilities and electronic properties of BC_2N sheets are intermediate between graphite (which is semimetallic) and BN (which is an insulator). In fact, conductivity measurements show that the BC_2N sheet is semiconductor with a band gap of ~0.03 eV.

Several possible arrangements for the BC_2N unit cell in monolayer have been suggested and studied. The relative stability of these geometries is believed to depend on the competition of structural stress and chemical bond strength. Figure 1 shows some two structures with lowest energies. Although it was initially thought that the **1a** structure is the most stable, subsequent studies showed that **1b** is more stable.

1a **1b**

Figure 1. Two possible configurations for the unit cell of hexagonal BC_2N sheets.

In this work we have studies the electronic properties of nanotubes formed by rolling a BC_2N sheet with the structure given in Figure 1b. Because of the anisotropy in the BC_2N sheets, two types of zigzag (ZZ-1 and ZZ-2) and two types of armchair (AC-1 and AC-2) nanotubes are possible for these compounds. We have studied a wide range of nanotubes from the four categories above and various diameters to investigate the dependence of electronic properties on the diameter and chirality of nanotubes. DFT-GGA calculations have been performed with plane waves and ultra-soft pseudopotentials implemented in Quantum Espresso software.

The results show that, except one case for a relatively small-diameter tube, all systems are semiconductors. The band gap ranges from 0.5 to 1.2 eV and various states of direct or indirect gaps are observed. In the limit of high diameters, the band gap is shown to be independent of the chirality and the values for all nanotubes fit on a same curve.

References:

1. S. Azevedo, Eur. Phys. J. B 44, 203-207 (2005).
2. S. Jalili, F. Molani, J. Schofield, Can. J. Chem. 91, 598-604 (2013).

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

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Due to the direct applicability of Ni(111) surfaces in high-quality graphene production, the Ni(111)-graphene interface has recently been the object of extensive experimental and theoretical investigations. Achieving an accurate and efficient theoretical description of the Ni(111)-graphene interaction, however, still represents a major theoretical challenge, due to the complex interplay between van der Waals (vdW) and hybridization effects.

Here we apply the DFT/vdW-WF2s method [1], augmenting semi-local Density Functional Theory through the inclusion of screened vdW interactions.

Interestingly, we show that a reliable description of the vdW energy in transition metals-graphene interfaces requires an appropriate modeling of the metal-screening, which should not only account for the p- and s-like ``quasi-free'' electrons, but should further include the effect of the more ``localized'' d-like states.

Good agreement is found with experiment and highly accurate theoretical predictions. Moreover, being the DFT/vdW-WF2s method based on Maximally Localized Wannier Functions, it permits an intuitive understanding of the complex physics underlying transition metals-graphene interactions. [1] P. L. Silvestrelli and A. Ambrosetti, Phys. Rev. B 87, 075401 (2013)

Electrostatics of solvated systems in periodic boundary conditions

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Continuum solvation methods can provide an accurate and inexpensive embedding of quantum simulations in liquid or complex dielectric environments. Notwithstanding a long history and manifold applications to isolated systems in open boundary conditions, their extension to materials simulations, typically entailing periodic boundary conditions, is very recent, and special care is needed to address correctly the electrostatic terms. We present how periodic boundary corrections developed for systems in vacuum should be modified to take into account solvent effects, using as a general framework the self-consistent continuum solvation model developed within plane-wave density-functional theory [O. Andreussi et al. J. Chem. Phys. 136, 064102 (2012)] and implemented in the Quantum ESPRESSO distribution. A comprehensive discussion of real- and reciprocal-space corrective approaches is presented, together with an assessment of their ability to remove electrostatic interactions between periodic replicas. Numerical results for zero- and two-dimensional charged systems highlight the effectiveness of the different suggestions, and underline the importance of a proper treatment of electrostatic interactions in first-principles studies of charged systems in solution.

Structural and electronic properties of Polyacetylene chains through Variational Monte Carlo

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The accurate description of the structural and electronic properties of π-conjugated molecules is still a challenge for many Quantum Chemistry methods, due to the necessity to give a balanced description of dynamical electronic correlation. Here we report the structural properties of polyacetylene chains, that are built from the repetition of $(C_2H_2)_N$ acetylene units, by means of the Variational Monte Carlo (VMC) method. In order to describe the electronic ground state, we use the Jastrow Antisymmetrized Geminal Power (JAGP) wave function, which is an ansatz able to properly describe the π-conjugation of these compounds. The reported Bond Length Alternation (BLA), namely the difference between the single and double carbon bonds, extrapolates, for $N \rightarrow \infty$, to a value of 0.0910(7) Å compatible with the experimental data. An accurate analysis was able to distinguish between the contributions of the Jastrow factor and of the AGP on the geometrical properties. Our results further demonstrate the possibility to obtain accurate reference structures of large molecules through Variational Monte Carlo.

Solvation effects on the color optical properties of anthocyanin natural dyes

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Anthocyanins are a class of natural dyes responsible for the vivid coloration of many flowers and fruits, and they are receiving a broad attention in the food industry, as food pigments, as well as in the drug industry as antioxidant agents. Here, we present a first-principles study of the dielectric and thermal-fluctuation effects on the color optical properties of these molecules upon solvation in water. Molecular configurations are first sampled via ab-initio molecular dynamics treating the solvent explicitly at room temperature [1]. Absorption spectra are then computed on the fly, using a recently proposed implicit-solvent model for the optical properties, based on a combination of the Liouville approach to time-dependent Density-Functional Theory [2,3] and the *Self-Consistent Continuous Model* [4,5] to describe the dielectric effects of solvation. When hybrid B3LYP/PBE0 exchange-correlation functionals are used, our treatment of the solvent results in an excellent agreement between simulated and experimentally observed spectra and colors in solution.

1. Malcioglu, O. B., Calzolari, A., Gebauer, R., Varsano, D., & Baroni, S. (2011). *J. Am. Chem. Soc. 133*, 15425.
2. Rocca, D., Gebauer, R., Saad, Y., & Baroni, S. (2008), *J Chem. Phys. 128*, 154105.
3. Ge, X., Binnie, S., Rocca, D., Gebauer, R., & Baroni, S. (2014), *Comp. Phys. Commun. 185*, 2080–2089.
4. Andreussi, O., Dabo, I., & Marzari, N. (2012), *J. Chem. Phys. 136*, 064102.
5. Timrov I., Andreussi O., Biancardi A., Marzari N., & Baroni, S. (2014), submitted.

Solution of the many-body problem in one point

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In this work [1] we determine the one-body Green's function as solution of a set of functional integro-differential equations, which relate the one-particle Green's function to its functional derivative with respect to an external potential. In the same spirit as Lani *et al.* [2] we do this in a one-point model, where the equations become ordinary differential equations and, hence, solvable with standard techniques. This allows us to analyze several aspects of these differential equations as well as of standard methods for determining the one-body Green's function that are important for real systems. In particular: i) We present a strategy to determine the physical solution among the many mathematical solutions; ii) We assess the accuracy of an approximate differential equation related to the GW+cumulant method by comparing it to the exact physical solution and to standard approximations such as GW; iii) We show that the solution of the approximate differential equation can be improved by combining it with a screened interaction in the random-phase approximation; iv) We demonstrate that by iterating the GW Dyson equation one does not always converge to a GW solution and we discuss which iterative scheme is the most suitable to avoid such errors.

[1] J.A. Berger, P. Romaniello, F. Tandetzky, B.S. Mendoza, Ch. Brouder, and, L. Reining, New J. Phys. 16,113025 (2014)
[2] G. Lani, P. Romaniello, and, L. Reining, New J. Phys. 14, 013056 (2012)

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

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Hydroxyapatite (HAp), with the chemical formula $Ca_{10}(PO_4)_6(OH)_2$, is the basic mineral constituent of human bone and tooth enamel. In stoichiometric HAp the Ca/P molar ratio is 1.67. However, HAp's constitution in human bones is usually nonstoichiometric and Ca-deficient with Ca/P ratio varying from 1.5 to 1.67. Since biological and mechanical properties of HAp are associated with Ca-deficiency, fundamental understanding of the defect chemistry and mechanical properties of Ca-deficient HAp is essential for not only understanding as to how nature works but also for designing synthetic biomaterials. Experimental investigation of the effect of calcium deficiency on mechanical properties of single crystals of HAp using nanoindentation, disclosed a striking 80% drop in its elastic modulus and hardness, and a marked 75% reduction in toughness, when Ca/P ratio changes from 1.67 to about 1.5. To gain insights into the mechanism of this degradation, we employ first-principles calculations based on density functional theory (DFT), and determine the effects of Ca deficiency on structure, vibrational and elastic properties of HAp.

Our estimated elastic constants of stoichiometric HAp agree well with experimental and theoretical results reported earlier. Calculated elastic constants reveal up to 30% reduction in the elastic constants and moduli of HAp due Ca-deficiency, and more such reduction is expected at higher strains and temperatures. Our calculations reveal the presence of a metastable state, for one of the defect structures considered, under applied pressure. We propose this as a cause for experimentally observed drastic reduction in the modulus and hardness for Ca-deficient HAp, seen in indentation experiment. Geometrical analysis of the local atomic structures of Ca-deficient HAps reveals the presence of hydrogen bonding in all the defect structures considered, consistent with the earlier experimental reports. Presence of weak hydrogen bonds in Ca-deficient HAp structures could also account for the degradation in the moduli due to Ca deficiency. Elastic anisotropic behavior of stoichiometric and Ca-deficient HAp is analyzed, which will be useful in understanding the effect of crystal orientation in designing synthetic bone. The defect formation energies are estimated for various defect structures under consideration and their electronic structures are compared with that of defect free HAp. Local structural stability of the defect structures assessed with full phonon spectra confirms the stability of all these structures including the reported metastable state. The comparative analysis of phonon frequencies of stoichiometric and Ca-deficient HAp structures, and the specific signatures in the computed vibrational spectra for Ca vacancies in HAp can be utilized in experimental characterization of Ca-deficient HAp.

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

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The known failure of the LDA/GGA approximation is the underestimation of the band gap in semiconductors and insulators. The band gap error can be corrected by the inclusion of the +U term for particular atomic orbitals [1]. While the impact of the +U term on bands of an ideal crystal was extensively discussed, its impact on the electronic structure of defects is less understood.

The +U correction was treated as a free parameter, and it was applied to both p(N) and transition metal d(TM) orbitals. We systematically analysed the effect of U on the properties of the gallium vacancy V:Ga, and of the Mn and Fe ions in GaN. The +U correction strongly affect the electronic structure of those centers, and, importantly, the GGA+U results are close to those obtained using the hybrid functionals [2,3,4]. Comparison with the available experimental data shows that U(N)=4 eV reproduces well the gap of GaN. Surprisingly, for U=0, the energies of the gap levels induced by the centers, and those of the intra-center optical transitions, agree well with experiment. In contrast, for U(N)=U(TM)=4 eV, the theoretical predictions are in substantial disagreement with experimental data by about 1-2 eV.

Supported by grants POMOST/2012-5/10 and NCN 2012/05/B/ST3/03095.

[1] M. Cococcioni and S. de Gironcoli, Phys. Rev. B **71**, 035105 (2005).
[2] A. Stroppa and G. Kresse, Phys. Rev. B **79**, 201201(R) (2009).
[3] P. Alippi, F. Filippone, G. Mattioli, A. A. Bonapasta, and V. Fiorentini, Phys. Rev. B **84**, 033201 (2011).
[4] R. Gillen and J. Robertson, J. Phys.: Condens. Matter **25**, 405501 (2013).

Koopmans' compliant functionals:

benchmarks on the G2 set,

photoemission spectra, and orbital reconstruction

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Koopmans-compliant functionals emerge naturally from extending the constraint of piecewise linearity of the total energy
as a function of the total number of electrons to each fractional orbital occupation.
When applied to approximate density-functional theory, these corrections give rise to orbital-density dependent functionals and potentials.

We show that these functionals, aiming at piecewise linearity against an external electron reservoir, provide accurate estimates for molecular quasiparticle excitations and leave the total energy functional almost or exactly intact, i.e., they describe correctly electron removals or additions, but do not alter the electronic charge density dis tribution within the system.
As such, Koopmans compliance can be applied to other self-interaction corrected functionals that modify the potential energy surface, e.g. according to the suggestion of Perdew and Zunger.
We discuss in detail these different formulations, and provide extensive benchmarks for the 55 molecules in the reference G2-1 set, using Koopmans-compliant functionals constructed from local-density or generalized-gradient approximations and their Perdew-Zunger counterparts.

In particular, the latter are both exactly one-electron self-interaction free, and approximately many-electron self-interaction free. In all cases we find excellent performance in the electronic properties, comparable or improved with respect to that of many-body perturbation theories, such as G0W0 and self-consistent GW, at a fraction of the cost and in a variational framework that also delivers energy derivatives.
These remarkable agreement extends also deeper into the spectral structure of molecules, and the agreement with UPS spectra is also very good.
Last, structural properties and atomization energies preserve or slightly improve theaccuracy of the underlying density-functional approximations.

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

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Even though it is the simplest element of the periodic table, hydrogen shows both a rich and complex behavior at high pressure. Metallic atomic hydrogen is expected at megabar pressures - metallization is expected at 450 GPa[1] -, which is predicted to show extraordinary properties such as high temperature superconductivity [2,3]. However, the theoretical study of such a light element as hydrogen turns out to be difficult due to the importance of nuclear quantum effects.

Here we present our *ab-initio* calculations of tetragonal $I4_1$/amd hydrogen, which is predicted to be its first atomic and metallic phase[4,5]. Our DFT calculations in the 400-500 GPa range show a nearly-free-electron-like metallic band structure. DFPT phonon calculations show a long-range behavior of lattice dynamics and Kohn anomaly-related softenings appear in some points of the first Brillouin zone. The phonon spectra calculated within the free electron Lindhard response show strong Kohn anomalies acting against the stability of the crystal. Furthermore, the anharmonic phonon spectra calculated with the SSCHA method [6] predict that anharmonic effects act against the stability of the system.

References:

[1] P. Loubeyre, F. Occelli, and R. LeToullec, *Nature* **416**, 613 (2002)

[2] N. W. Ashcroft, *Phys. Rev. Lett*. **21**, 1748 (1968).

[3] P. Cudazzo, G. Profeta, A. Sanna, A. Floris, A. Continenza, S. Massidda, and E. K. U. Gross, *Phys. Rev. Lett.* **100,** 257001 (2008).

[4] J. M. McMahon and D. M. Ceperley, *Phys. Rev. Lett.* **106**, 165302 (2011).

[5] S. Azadi, B. Monserrat, W. M. C. Foulkes, and R. J. Needs, *Phys. Rev. Lett*. **112**, 165501 (2014).

[6] I. Errea, M. Calandra, and F. Mauri, *Phys. Rev. Lett.* **111**, 177002 (2013).

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

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The description of charge transfer in organic structures has long been a challenge to Density Functional Theory (DFT) based methods. The recently developed concept of "tuned range separated functionals" has proven to describe charge transfer accurately in many cases. However, describing solvated or embedded systems is yet a challenge. We discuss how such systems can (or cannot) be coped with on a first-principles DFT basis. Combining DFT and molecular dynamics simulations we quantitatively predict the influence of molecular distortions and solvation effects on the optical gap of paradigm oligomers, and we discuss approaches for a reliable description of realistic systems.

Light-induced field enhancement in polyacenes

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Carbon-based nanostructures, such as graphene nanoribbons and nanoflakes, have been studied in the past years for their unique electronic, mechanical and thermal properties. High attention has been devoted recently to their optical, absorption and plasmonic properties, in view of possible applications as sensors, amplifier antenna and light harvesting devices [1]. Plasmonic properties of bulk metals (e.g. Au, Ag) have been known for a long time, and recently these concepts have been extended to carbon nanostructures [2]. Scaling down from macro- to the nano-scale the optical properties of nano-systems do not have a well defined character as in the bulk and are more complicated to be characterized. In particular, the way the excitation properties of molecules transform into that of nanostructures and then into macroscopic bulk is far from being understood, and it is a field of great current interest.

Here, we take into account polyacenes with a number of rings between 1 and 5 and the 50-acene. Moreover we consider coupled acenes (naphthalenes) at different distances. Their electronic and optical absorption properties and the local electric field enhancement near them are investigated through state-of-the-art (TD)DFT first-principles approaches [3] with particular emphasis on their scaling with respect to the size of the system and the intermolecular distance, in the case of the dimers [4].

The analysis of the dominant band-to-band single-particle transitions in the lowest energy excitations of acenes leads to the identification of the main peak in the UV-vis TDDFT optical spectra as a collective "molecular plasmon" resonance [5]. The resulting confinement of electromagnetic energy to nanometric regions can produce a local enhancement of the external electromagnetic field near the nanosystem, thus acting as an optical nanoantenna. The plasmonic character of different excitations is also discussed. While the amplification of the electric field in the vicinity of single acenes decreases when the size of the system is increased, it may be selectively enhanced in the case of acenes' assemblies. This proof of concept suggests that supramolecular coupling may provide a tunable way to realize realistic nanoantenna and paves the way for the design of more complex C-based architectures, explicitly conceived to enhance the amplification factor.

References

[1] (a) E. Ozbay, *Science*, **311**, (2006) 189; (b) M. Brongersma, V. Shalaev, *Science*, **328**, (2010) 440.
[2] A. Manjavacas, et al., *ACS NANO*, **7**, (2013) 3635.
[3] (a) P. Giannozzi, et al. *J. Phys.: Condens. Matter,* **21**, (2009) 395502. See also www.quantum-espresso.org; (b) D. Rocca, et al., *J. Chem. Phys.,* **128**, (2008) 154105.
[4] L. Bursi et al., *ACS Photonics*, **1**, (2014) 1049.
[5] S. Bernadotte, F. Evers, and C. R. Jacob, *J. Phys. Chem. C*, **117**, (2013) 1863.

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

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Noble metals are conventionally used as plasmonic building blocks in the fields of the telecommunications and energy conversion. Both localized surface plasmons in nanoparticles and surface plasmon polaritons (SPP) at metal/semiconductor interfaces are of interest for optoelectronic applications: the formers can be exploited in photovoltaic systems as amplifier antenna; the latters provide the opportunity of confining and propagating light over long spatial range [1].

However, metals are plagued by large losses in the UV–vis and IR spectral ranges, arising from interband transitions and dissipative scattering events. As an alternative, heavily doped semiconductors, such as transparent conductive oxides (TCOs), can exhibit a small negative real permittivity and very small losses at the infrared and longer wavelengths [2].

Using first principles calculations, we investigate the origin of near-infrared plasmonic activity in Al-doped ZnO (AZO), one of the most promising indium-free TCO materials for optoelectronics and photovoltaics applications. Our results [3-4] predict realistic values for the plasma frequency and the free electron density as a function of the Al-doping, in agreement with recent experimental results. Then, we show the formation of SPP at the AZO/ZnO interfaces in terms of characteristic lengths that can be measured by experiments. These systems present tunable plasmonic activity in the near-IR range and in particular at wavelength also relevant for telecommunications (1,5 μm) [3].The direct comparison with standard plasmonic metals underlines the promising capabilities of TCOs as compact and low-loss plasmonic materials for energy conversion applications and telecommunications.

[1] W.A. Murray et. al , Adv. Mater. 19, 3771 (2007).
[2] G.V. Naik, G. V., Adv. Mater. 25, 3264 (2013).
[3] A. Calzolari, et al., ACS Photonics 1, 703 (2014).
[4] M. Bazzani, et al., Appl. Phys. Lett. 98, 121907 (2011).

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

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Chalcogenide alloys such as the $Ge_2Sb_2Te_5$ (GST) and GeTe compounds are of interest for applications in non-volatile phase change memories (PCM) thanks to their ability to undergo a fast and reversible phase transformation between the crystalline and amorphous phase upon heating [1]. The set and reset of the memory correspond to the recrystallization of the amorphous phase and to the melting and subsequent amorphization of the crystal induced by Joule heating. Thermal conduction is a key factor for the device operation, as the set/reset processes strongly depend upon heat dissipation and transport. Thermal boundary resistance (TBR) at the interface between GST and the surrounding dielectrics and metallic electrodes is another crucial parameter for the control of thermal crosstalks with adjacent cells which may arise during memory programming. A large TBR can also lead to a reduction in the programming current thanks to heat confinement effects [2]. In this contribution, we report on density functional calculations [3] of the bulk thermal conductivity in crystalline GST that allowed us to identify the source of scattering responsible for the glass-like thermal conductivity of this crystal. Thermal boundary resistance at different interface of crystalline GST and GeTe with dielectrics and metals have been estimated from ab-initio phonons and the Diffuse Mismatch Model [4]. The calculations revealed that an important contribution to the TBR comes from the electron-phonon coupling [5] within GST and GeTe. For the amorphous/crystalline interface, which is also present in the device, we used an interatomic potential generated with a Neural Network method [6] and non-equilibrium molecular dynamics simulations [7]. This work provides a comprehensive analysis of the different source of thermal resistance of great value for a reliable electrothermal modelling of the memory device.

[1] M. Wuttig and N. Yamada, Nature Materials **6**, 824 (2007).
[2] J. P. Reifenberg, K.-W. Chang, M. A. Panzer, S. Kim, J. A. Rowlette, M. Asheghi, H.-S. P. Wong, and K. E. Goodson, IEEE Elect. Dev. Lett. **31**, 56 (2010).
[3] L. Paulatto, F. Mauri and M. Lazzeri, Phys. Rev. B **87**, 214303 (2013).
[4] G. Chen, Phys. Rev. B **57**, 14 958 (1998).
[5] A. Majumdar and P.Reddy, Appl. Phys. Lett. **84**, 4768 (2004).
[6] G. C. Sosso, D. Donadio, S. Caravati, J. Behler, and M. Bernasconi, Phys. Rev. B **86**, 104301 (2012).
[7] F. Muller-Plathe, J. Chem. Phys. **106**, 6082 (1997).

Surface-assisted formation of grapheme nanoribbons on Au surfaces

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The formation of graphene nanoribbons (GNRs) on Au(110) and Au(111), as based on the surface mediated reaction of 10,10'-dibromo-9,9' bianthracene (DBBA) molecules was investigated by means of first-principles calculations. The study was done in direct collaboration with experimental groups performing structural and spectroscopic characterization by means of STM, XPS/UPS, NEXAFS.

Comparison between the Au(110) and Au(111) surfaces unveils the delicate interplay between surface atomic corrugation, molecular mobility, and adsorption energies, that drive the GNR growth. Concerning the Au(110) surface, we have studied the molecule/surface interaction at different stages of the GNR formation. The role of different reconstructions has been investigated, showing that both precursors and GNRs interact differently with different surfaces. Calculations for the precursor molecules showed that initial stages of the reaction crucially determine the final configuration and orientation of the GNRs. In the specific case of Au(111) we have also studied the evolution of the Au Shockley surface state as a function of GNR growth [1]. We show that the GNR/Au interaction results in an upshift of the Shockley surface state of Au(111) by 0.2 eV, together with an increased electron effective mass in very good agreement with the experimental findings.

[1] A. Batra, D. Cvetko, G. Kladnik, O. Adak, C. Cardoso, A. Ferretti, D. Prezzi, E. Molinari, A. Morgante, L. Venkataraman, Chem. Sci., 5, 4419, 2014

Electron energy loss anisotropies in MAX phases: Ti_2AlC

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The MAX phases are a new class of ternary compounds that exhibit an unusual combination of ceramic and metallic properties [1]. Their composition can be written $M_{n+1}AX_n$ where M stands for an early transition metal, A for a metal of the group A like Al, S, Ge and X is C or N. Their crystallographic structure is highly anisotropic with a c/a ratio exceeding 4.5 and consists of alternating layers of carbide or nitride units and A-element layers. This specific structure is partly responsible for their unique properties [2].

In the present work we address the calculation of the electron energy loss function for Ti_2AlC chosen as example of these compounds. Previous calculations of the EEL spectra for vanishing momentum transfer of Ti_2AlC indicate a very strong anisotropy in the spectra obtained for different crystal orientation. Additionally they show an important influence of crystal local-field effects in the c-axis direction, while they are practically negligible parallel to the base plane [3]. These finding motivated us study the non-zero momentum transfer of Ti_2AlC using TDDFT-RPA and ALDA. Coherently with the vanishing momentum results, we find a strong anisotropy and different effect of local fields for momentum transfer oriented along the basal plane and along the c-axis. In addition we discuss the plasmon dispersion.

[1] Die H-Phasen: Ti_2CdC, Ti_2GaC, Ti_2GaN, Ti_2InN, Zr_2InN and Nb_2GaC, W. Jeitschko, H. Nowotny, and F. Benesovsky, Monatsh. Chem. **95**, 431 (1964).

[2] The $M_{N+1}AX_N$ Phases: A New Class of Solids; Thermodynamically Stable Nanolaminates, M.W. Barsoum, Prog. Solid. State. Chem. **28**, 201 (2000).

[3] Dielectric properties of Ti_2AlC and Ti_2AlN MAX phases: the conductivity anisotropy, N. Haddad et al., J. of Appl. Physics **104**, 023531 (2008).

Phonon Hydrodynamics in Two-Dimensional Materials

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We characterise the thermal conductivity of two-dimensional materials, such as graphene, molybdenum disulphide and others, by solving the Boltzmann Transport Equation (BTE) for phonons [1], with the phonon-phonon collision rates obtained from density-functional perturbation theory. A self consistent, exact solution of the equations allows us to show that heat transport in the examined materials can only be explained in terms of collective phonon excitations [2]: heat is frequently exchanged between phonon modes but only rarely dissipated, due to the dominance of heat-flux conserving Normal scattering events. This behaviour, which has been observed to date only in few large crystals free of defects at cryogenic temperatures, is present in two-dimensional materials at room temperature. As a consequence, exotic phenomena need to be considered, as the description of the heat-flux as the flow of a fluid, and the appearance of second sound.

[1] M. Omini and A. Sparavigna, Nuovo Cimento D 19, 1537 (1997)

[2] G. Fugallo et al., Nano. Lett., 14, 6109 (2014)

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

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We consider an ensemble of ultra-cold alkali atoms trapped in a periodic lattice with all valence electrons in highly excited overlapping orbitals of principal quantum number n. Possible implementations of this system in nanoplasmonic [1] or optical [2] lattices, realize an extremely dilute electron gas where exchange and correlation energies dominate over the kinetic energy.

We characterize the basic electronic structure properties in this regime within the homogeneous electron gas approximation and present first results based on density functional theory (DFT). DFT calculations were performed with the plane-wave Quantum-Espresso code [3] and special norm-conserving pseudopotentials developed by us to simulate a long-living highly excited alkali atom (Rydberg atoms).

We calculate the equilibrium lattice constant as a function of the principal quantum number n and the band structure at the single-particle level, which will be the starting point for including many-body effects beyond DFT. Finally, we discuss the stability of the system with respect to radiative and Auger decay processes.

[1] M. Gullans et al., Phys. Rev. Lett. **109**, 235309 (2012).
[2] M. Greiner et al., Nature **415**, 39 (2002).
[3] P. Giannozzi et al., J. Phys. Cond. Mat. **21**, 395502 (2009).

Designing FePt-Fe_3Pt hard-soft magnetic composite materials from *ab initio* calculations

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The challenge of finding strong rare-earth free permanent magnets includes the design and discovery of new hard magnets. A composite with a soft magnet of high saturation magnetization and a hard magnet of high coercive field may exhibit strong exchange coupling which may result in large coercivity as well as high magnetic moments. Among many promising rare-earth free candidates, FePt with tetragonally distorted face centered cubic (FCC) structure is a hard magnet with strong magnetic crystalline anisotropy. The Fe_3Pt phase has perfect FCC structure and is a soft magnet. A combination of FePt and Fe_3Pt forms an exchange-coupled strong magnet. Experimentally, FePt-Fe_3Pt nanocomposite has been shown to have high energy product (20.1 MGOe) compared to single phase FePt (14.7 MGOe). The magnetization and anisotropy properties of these nanocomposites mainly depend on two factors: (i) The interfacial conditions which could lead to high magnetic moments due to strong exchange-coupling between soft and hard magnets and (ii) the thickness of the hard/soft magnet in the nano-composite. Our studies on small Fe-Pt clusters and medium size nanoparticles have shown large magnetic moments ($>3\mu_B$) on Fe atoms, enrichment of Pt at low coordination sites, and maximization of unlike bonds. This led us to design an icosahedral $Fe_{75}Pt_{72}$ nanoparticle with almost equal composition of Fe and Pt. The magnetic moments on Fe atoms below the surface have about 3 μ_B value while the surface atoms have a value higher than 3 μ_B. We report here results on FePt-Fe_3Pt hard-soft magnetic composites including nanoparticle composite as well as superlattices using PAW pseudopotential method and spin-polarized GGA for the exchange-correlation energy. The interfacial conditions and the effect of the thickness of FePt/Fe_3Pt on magnetic moments have been explored. We find that the hard magnet FePt imposes face centred tetragonal symmetry on Fe_3Pt which signifies strong structural anisotropy. The magnetic moments are enhanced from their bulk phase values. The depletion/excess concentration of Fe/Pt in different regions plays a key role in the advancement of the magnetic properties of the composite.

We thankfully acknowledge the staff of CDAC, Pune for the use of computer resources as well as HPC resources at Shiv Nadar University and AOARD for financial support.

Searching for high magnetization density in bulk Fe: the new metastable Fe_6 phase

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In this poster we report the discovery of a new allotrope of iron by first principles calculations. This phase has $Pmn2_1$ symmetry, a six-atom unit cell (hence the name Fe_6), and the highest magnetization density (M_s) among all known crystalline phases of iron. Obtained from the structural optimizations of the Fe_3C-cementite crystal upon carbon removal, $Pmn2_1$ Fe_6 is shown to result from the stabilization of a ferromagnetic FCC phase, further strained along the Bain path. Although metastable from 0 to 50 GPa, the new phase is more stable, at low pressures, than the other well-known HCP and FCC allotropes and smoothly transforms into the FCC phase under compression. If stabilized to room temperature, e.g., by interstitial impurities, Fe_6 could become the basis material for high M_s rare earth-free permanent magnets and high-impact applications such as, light-weight electric engine rotors or high-density recording media. The new phase could also be key to explain the enigmatic high M_s of $Fe_{16}N_2$, which is currently attracting an intense research activity.

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

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Scanning tunnelling spectroscopy (STS) visualizes electron states in both extended systems and nano-objects, such as molecules. When the molecule is weakly coupled to the substrate, its states keep their molecular identity and remain well-separated in energy. Electrons (or holes) incoming from the STS tip, tunnel to the substrate through such molecular states. Under this Coulomb blockade-like condition, STS maps the wave function modulus of the electron/hole injected by the tip into the molecule. The obtained image is routinely interpreted as the molecular orbital [1] of the added electron/hole, that experiences the mean field of the other electrons already populating the system. A fundamental question is whether features of the tunnelling map may appear due to electron-electron correlation beyond mean field in this molecular regime[2].

In this work [3] we demonstrate that the STS images of single planar molecules with metal centres predicted by ab initio many-body calculations differ qualitatively from their uncorrelated counterparts. We find in the STS maps resolved at the Fermi energy that correlation alters significantly the spectral weight around the metal atom. This change may be experimentally quantified by contrasting the altered STS images to those of substituted molecules unaffected by correlation that are used as benchmarks.

[1] J. Repp, G. Meyer, S. M. Stojkovic, A. Gourdon, and C. Joachim, Phys. Rev. Lett. **94,** 026803 (2005).
[2] M. Rontani and E. Molinari, Phys. Rev. B **71,** 233106 (2005); M. Rontani, Nature Mat. **10,** 173 (2011).
[3] D. Toroz, M. Rontani, and S. Corni, J. Chem. Phys. **134,** 024104 (2011); Phys. Rev. Lett. **110,** 018305 (2013).

DFT study of the reactivity of CO_2 in molten alkali carbonates

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Our theoretical study is carried on in the context of a project that focuses on an original route to tackle the challenging problem of CO_2 sequestration and re-use. The idea is to employ molten carbonates, commonly used electrolytes in fuel cells, due to their ability to dissolve CO_2 (see for example [1]). To this aim, the nature and composition of the carbonate melt have to be optimized for CO_2 dissolution and reduction. A crucial step in this direction is to gather new data on the solvation and transport of CO_2 in molten carbonates and get a better understanding of these processes at the molecular level. By DFT first principles molecular dynamics simulations we study the properties of the solvent melt Li_2CO_3-K_2CO_3 at the eutectic ratio (62:38%) at three different temperatures, T = 900, 1000, 1100 K. Then the solvation of CO_2 in the melt is investigated with particular focus on the possible formation of the pyrocarbonate ion $C_2O_5^{2-}$. This species was observed in the gas phase [2, 3] and, albeit short-lived, in the condensed phase of $CaCO_3$ [4]. Furthermore, it has been observed that the solubility of CO_2 in the carbonates increases with increasing temperature, a fact that seems to contradict the exothermic nature of the formation reaction of $C_2O_5^{2-}$ in the gas phase. It is then necessary to ascertain what is effect of the environment in the condensed phase. Preliminary results indicate that the pyrocarbonate ion is quite stable in the eutectic Li_2CO_3-K_2CO_3 melt, with possible implications on the thermodynamics of reactivity and on the transport of CO_2 in this particular melt.

[1] D. Chery, V. Albin, V. Lair & M. Cassir, *Thermodynamic and experimental approach of electrochemical reduction of* CO_2 *in molten carbonates*. Int. J. Hydrogen Energ. **39**, 12330 (2014).

[2]. D. Peeters, D. Moyaux & P. Claes, *Solubility and Solvation of Carbon Dioxide in the Molten* $Li_2CO_3/Na_2CO_3/K_2CO_3$ (43.5:31.5:25.0 mol-%) *Eutectic Mixture at* 973 K. II. *Theoretical Part*. Eur. J. Inorg. Chem. **1999**, 589 (1999).

[3] P. J. Bruna, F. Grein & J. Passmore, *Density functional theory* (DFT) *calculations on the structures and stabilities of* $[C_nO_{2n+1}]^{2-}$ and $[C_nO_{2n+1}]X_2$ *polycarbonates containing chainlike* $(CO_2)_n$ *units* (n = 2–6; X = H or Li). Can. J. Chem. **89**, 671 (2011).

[4] R. Vuilleumier, A. Seitsonen, N. Sator & B. Guillot, *Structure, equation of state and transport properties of molten calcium carbonate* (CaCO3) *by atomistic simulations*. Geochim. Cosmochim Ac. **141**, 547 (2014).

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

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We present a first-principle investigation of the fully relativistic electronic surface states and resonances of the clean Pt(111) and Ir(111) surfaces and compare them with those of Au(111).[1] Our calculations are based on a recently introduced fully relativistic projector augmented-wave (PAW) [2] approach that includes spin-orbit coupling and allows us to access both the relativistic energy splittings and the spin polarization of the surface states. The maps of the electronic structure of the two surfaces are critically discussed in comparison with previous calculations and with some of the available angle-resolved photoelectron spectroscopy data.

[1] R. Mazzarello, A. Dal Corso, and E. Tosatti, Spin-orbit modifications and splittings of deep surface states on clean Au(111), Surf. Sci. **602**, 893 (2008).
[2] A. Dal Corso, Projector augmented-wave method: application to relativistic spin-density functional theory, Phys. Rev. B **82**, 075116 (2010).

First-principles study of Radical Organic Electrodes

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During the last decade, organic polymers bearing stable redox-active radical pendant groups have been identified as promising materials for secondary batteries. These organic radical electrodes present valuable features such as low-cost, abundant, lightweight and furthermore their electronic properties can be rationally tuned.

The most studied radical compounds for electrode applications are nitroxide based polymers. Nitroxide can be reversibly n-doped to aminoxyl anion and p-doped to oxoammmonium cation in anodic and cathodic reaction, respectively. Poly(2,2,6,6-tetramethyl-1-piperidinyloxy-4-yl methacrylate) (PTMA) is the most common active material which has already been used as a cathode in Li-ion cells. It displays a reversible redox process around 3.6 V vs Li/Li+ with a theoretical capacity of 111 mAh/g.

The molecular engineering of new radical materials with tunable electrochemical properties could be guided by high-throughput ab initio calculations. As a first step in order to identify these original organic electrodes with predictive computational chemistry, we test the agreement between theoretical and experimental data for various organic radical polymers used as active materials in batteries.

Density functional theory relying on the B3LYP exhange-correlation functional is used to estimate the open cell voltage of Li-ion batteries using nitroxide radical bearing polymers. The solvation of the organics compounds is simulated by the SMD model [1] as implemented in the Gaussian09_D01 software [2]. The effect of counter anions and cations are examined for different solvents depending on the electrolyte salt. The results indicate that the method is sufficiently robust to extrapolate to theoretically designed nitroxide radicals.

[1] A. V. Marenich, C. J. Cramer, and D. G. Truhlar, "Universal solvation model based on solute electron density and a continuum model of the solvent defined by the bulk dielectric constant and atomic surface tensions," J. Phys. Chem. B, 113 (2009) 6378-96.

[2] Gaussian 09, Revision **D.01**, M. J. Frisch, et al., Gaussian, Inc., Wallingford CT, 2009.

On the interpretability of molecular orbitals from organic semiconductors

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Molecular orbitals (MO) serve as indispensable helpers for understanding quantum systems and their properties such as charge transfer and binding mechanisms. However, their physical significance cannot be taken for granted due to their auxiliary nature. Here, angle resolved photoemission (ARPES) has proved to be a powerful tool to probe the MO picture as it allows visualizing outer valence orbital densities of organic semiconductors. Since ARPES is formally related to the Dyson orbitals, we investigate in how far Kohn-Sham (KS) orbitals correspond to Dyson orbitals, and can thus truthfully predict photoemission experiments. As a first approach we investigate whether and under which conditions KS orbitals can be accurate one-to-one approximations to Dyson orbitals.

In a further step we use that the Dyson orbital actually emerges as the generalized overlap of the initial and the ionized ground state many-body wavefunction. We follow this approach, yet approximate the wavefunctions as KS-Slaterdeterminants and include molecular relaxation effects by using self consistently calculated orbitals for the neutral and the ionized system. The Dyson orbital is then written as a weighted sum over all initially occupied KS orbitals. We show that the Dyson orbital is dominated by the Kohn-Sham HOMO when relaxation effects are small, or when they are covered to a certain extent by the used exchange-correlation-functional. In particular, orbitals from a Kohn-Sham self-interaction-correction match the experimental spectra in all studied cases.

Addionally, we address APRES by a real-time simulation with time-dependent density-functional theory. This allows us to go beyond the static approximation and in particular to gain ARPES spectra without relying on the interpretation in terms of single orbitals.

Transport Properties of Iron-Porphyrin / Graphene Junction

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Spintronics is one of the possible applications of graphene-based materials [1]. To this end, a robust spin polarization in the graphene layers is required. This can be achieved via functionalization with magnetic transition metals, adsorbates, or organic molecules. It has been demonstrated that a Fe atom incorporated in the graphene network replacing a carbon-carbon dimer and bound to substitutional N atoms forms an almost-planar stable structure with notable magnetic properties [2].

In this work we study by first principles a Fe-Porphyrin molecule (FeP) embedded in a graphene nanoribbon junction connected with two semi-infinite graphene regions using the density functional theory (DFT) as implemented in the SIESTA package [3]. The analysis of the spectral properties shows a rearrangement of the orbital occupancy with respect to the isolated FeP molecule, while the magnetic moment remains unchanged ($2\mu_B$). The Fe $3d_{xz}$ and $3d_{yz}$ orbitals of both spin components hybridize with the carbon π bands. The other *d* states, due to their different parity, remain unperturbed.

We also investigate the interaction of a carbon monoxide molecule with the Fe atom. CO adsorbs with the carbon atom facing the metal center. The interaction is strong enough to be stable at room temperature, amounting to about 2 eV. The adsorption of CO modifies the occupancy of the Fe 3*d* states and totally quenches the magnetic behavior of the system.

We explore the effects of CO adsorption on the electronic transport properties calculating the transmission coefficient T(E) and the electric current in both cases. The calculations were performed using the TranSIESTA code [4], which combines the non-equilibrium Green's function (NEGF) technique with DFT. At zero bias the T(E) of the FeP junction does not significantly differ from that of pure graphene, except for a small perturbation at 0.1 eV below E_F in the minority component due to the hybridized $3d_{xz}$ Fe state, which for higher voltages becomes more evident. Consequently, the currents of the two spin components are different giving a polarization of 5%. When the CO molecule is adsorbed, the magnetic character of the system vanishes and the current becomes unpolarized.

This suggests the use of the current measurement as a possible tool for the detection of the adsorption of a CO molecule: both the disappearance of spin polarization or the decrease of the total current are evidences of the presence of this gas.

References

[1] O.V. Yazyev, M.I. Katsnelson, *Phys. Rev. Lett.* **100,** (2008) 047209.
[2] A.T. Lee, J. Kang, S. Wei, K,J. Chang, and Y. Kim, *Phys. Rev. B* **86**, (2012) 165403.
[3] J.M. Soler, E. Artacho, J.D. Gale, A. García, J. Junquera, P. Ordejón, and D. Sánchez-Portal, *J. Phys.: Condens. Matter* **14,** (2002) 2745.
[4] M. Brandbyge, J.-L. Mozos, P. Ordejón, J. Taylor, and K. Stokbro, *Phys. Rev. B* **65,** (2002) 165401.

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

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Stiffness tensors are thermodynamic quantities that provide a full characterization of the mechanical response of crystals in the linear regime of stress-strain. The prediction of their thermal dependence from empirical potentials can provide important tests for the validation of the model parametrization used to mimic the underlying electronic interactions. In this work, we investigate the thermoelastic properties of α-iron, first using selected embedded-atom potentials commonly used in the scientific community ([1],[2],[3],[4]). The temperature dependence of the stiffness tensor components, namely the elastic constants, is achieved via calculation of the change in the slope of the acoustic phonon modes in Γ obtained from NVT molecular dynamics runs. Our results show how, beyond the expected agreement with experimental data at low temperature (these data are included in the fitting training set), the reliability of the potentials become questionable in the high temperature regime.

Second, we investigate the same thermoelastic properties using first-principles total-energy and lattice-dynamics calculations, minimizing the quasi-harmonic Helmholtz free energy under finite strain deformations. Interestingly, the calculated elastic constants display a very good agreement with the experimental thermal behavior while showing significant discrepancies (14%, 20%, -15%, for B, C_{11}, C_{44} respectively) with respect to experiments at zero temperature. Possible reasons for these discrepancies can be attributed to the presence in the experimental monocrystalline samples of magnetic domain walls not considered in our calculations or to limitations of standard DFT approaches in treating *d*-electrons and magnetism. In the latter case, one could try to employ more complex methods (such as DFT+U+J, DMFT, RPA) to explore possible improvements in the description of the 0 K mechanical properties of α-iron.

1. M.I. Mendelev, S. Han, D.J. Srolovitz, G.J. Ackland, D.Y. Sun and M. Asta, Philos. Mag. 83, 3977 (2003)
2. R. Meyer and P. Entel, Phys. Rev. B 57, 5140 (1998)
3. Y. Ouyang, X. Tong, C. Li, H. Chen, X. Tao, T. Hickel, and Y. Du, Physica B 407, 4530 (2012)
4. M. Marchese, G. Jacucci, and C. P. Flynn, Philos. Mag. Lett. 57, 25 (1988)

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

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Describing vibrations of atoms is of paramount importance in the physical properties of solids. Nowadays, phonon dispersions in the harmonic approximation are routinely calculated from first-principles. Nevertheless, whenever the displacements of the atoms largely exceed the range in which the harmonic potential is valid, the harmonic approximation completely fails.

Here we present a newly developed approach to treat strongly anharmonic systems named as the stochastic self-consistent harmonic approximation (SSCHA) [1,2]. The method is variational and takes into account quantum and thermal effects rigorously. Moreover, it can be combined with third-order perturbation theory to calculate phonon lifetimes and spectral functions in strongly anharmonic crystals. Remarkably, the combination of these two methods yields the correct perturbative limit, but avoiding the cumbersome calculation of fourth-order force constants.

We demonstrate the validity of the SSCHA applying it to metallic hydrides and transition metal dichalcogenides.

[1] Ion Errea, Matteo Calandra, and Francesco Mauri, PRL 111, 177002 (2013)
[2] Ion Errea, Matteo Calandra, and Francesco Mauri, PRB 89, 064302 (2014)

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

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Checking the convergence of accuracy parameters (e.g. basis set), in ab initio molecular dynamics, is complicated and computationally expensive. This is because entire simulations are required for each new parameter set, and comparing two simulations is subject to large statistical errors in structural (pair correlation functions) and thermodynamic (pressure, compressibility) properties. In this work we propose a method to evaluate parameter convergence without these costly simulations. In the spirit of thermodynamic integration approaches, the average change of a given property is computed with different parameters in the same geometries, extracted from a given MD trajectory or set of trajectories. This same approach can be used to explore tendencies for new exchange-correlation functionals, so that only the most promising ones need to be thoroughly evaluated with entire simulations.

Thermoelectric properties of n-doped Silicon from first-principles

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Understanding dissipative and transport phenomena in semiconductors is a key task to design and engineer materials for thermoelectric and nano-electronic applications. Despite the exstensive activity in the field, the state-of-the-art still lacks a comprehensive first-principles numerical framework to tackle the problem.

Here we present a computational infrastructure to calculate the electronic transport coefficients of bulk systems within the Boltzmann transport equation (BTE) formalism. The electronic and vibrational properties, including the electron-phonon interaction, are computed using Density Functional theory and Density Functional Perturbation theory. We exploit the Wannier interpolation to efficiently sample fine grids in reciprocal space. The linearized BTE is solved exactly using a Conjugate Gradient algorithm. Our method goes beyond the standard practice, which relies upon various flavors of the relaxation-time approximation and makes use of semi-empirical models of carriers' dispersions and interactions.

We have applied this framework to study the thermoelectric properties of n-doped Silicon in a wide range of temperatures and doping concentrations. Our results are in good agreement with the experimental observations and elucidate the relative importance of the various scattering mechanism in the different regimes. As an additional outcome, we assess the accuracy of simplified models and approximations that are commonly used to study transport in semiconductors.

A generalized Poisson solver for complex electrostatic environments

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The computational study of chemical reactions in complex, wet environments is critical for applications in many fields, and of cross-disciplinary interest to physics, chemistry, materials science, chemical engineering, and biology [1]. It is often essential to study chemical reactions in the presence of an applied electrochemical potentials, establishing the correct relation between charge and potential, and taking into account the complex electrostatic screening coming from the solvent and the electrolytes [2]. In the present work we proposed an algorithm, based on the Preconditioned Conjugate Gradient (PCG) method, to handle the Generalized Poisson equation. It allows to solve iteratively the minimization problem with some ten iterations. The algorithm takes advantage of a preconditioning procedure which exactly represents the operator in the limit of a slowly varying dielectric constant, and is based on the BigDFT Poisson solver for the standard Poisson equation [3,4]. The code turns out to be no-memory consuming and fast. The use of the BigDFT solver as preconditioner allows to manage free, surface, wire and periodic conditions. Applications of the generalized solver and comparison to other approaches will be presented which demonstrate the efficiency of the method.

[1] I. Dabo, N. Bonnet, Y. Li, and N. Marzari Ab-initio electrochemical properties of electrode surfaces. In A. Wieckowski and J. Norskov, editors, *Fuel Cell Science: Theory, Fundamentals and Bio-Catalysis.* John Wiley and Co. (2011).

[2] O. Andreussi, I. Dabo, and N. Marzari *J. Chem. Phys.* **136**, 064102 (2012).

[3] L. Genovese, T. Deutsch, A. Neelov, S. Goedecker, and G. Beylkin *J. Chem. Phys.* **125**, 074105 (2006).

[4] L. Genovese, T. Deutsch, and S. Goedecker *J. Chem. Phys.* **127**, 054704 (2007).

Anchoring and Bending of Pentacene on Aluminum (001)

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We study the structural, electronic, and spectroscopic properties of pentacene adsorbed on Al(001) surface, combining density functional theory (DFT) methods including van der Waals interactions with x-ray photoemission (XPS), near-edge x-ray absorption fine structure (NEXAFS), and scanning tunneling microscopy (STM). We find a major change of the molecular backbone resulting into a peculiar V-shape bending, due to the direct anchoring of the two central carbons atop two Al atoms underneath. In the most stable adsorption configuration, pentacene is oriented with the long axis parallel to the substrate [110] direction, where such anchoring is favored by optimally matched interatomic distances. Remarkably, due to the generally low degree of order, we measure by STM a significant portion of molecules oriented along the [100] direction, which also display the same V-shape conformation, as driven by the link of the central carbon atoms of pentacene to a pair of slightly displaced Al atoms.

Enhanced Atom Mobility on the Surface of a Metastable Film

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A remarkable enhancement of atomic diffusion is highlighted by scanning tunneling microscopy performed on ultrathin metastable body-centered tetragonal Co films grown on Fe(001). The films follow a nearly perfect layer-by-layer growth mode with a saturation island density strongly dependent on the layer on which the nucleation occurs, indicating a lowering of the diffusion barrier. Density functional theory calculations reveal that this phenomenon is driven by the increasing capability of the film to accommodate large deformations as the thickness approaches the limit at which a structural transition occurs. These results disclose the possibility of tuning surface diffusion dynamics and controlling cluster nucleation and self-organization [Phys. Rev. Lett. 2014, 113, 046102].

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

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We measure direct multiphoton photoemission of the Au(111) surface state with 800-nm laser pulses. We observe the parabolic dispersion in the angular distribution of photoelectrons having absorbed between four and seven photons. The k‖ dispersion we measure can be explained in terms of Shockley-state replicas, with a nascent hot electrons distribution at k‖ above the Fermi level. Moderate laser power densities, of the order of 100GW/cm2, resulted in large electron yields, indicating the importance of multiphoton excitations to define the electronic and magnetic properties of matter in the first hundred femtoseconds after laser excitation [Phys. Rev. B 2014, 90, 035401].

Resonant Lifetime of Core-Excited Organic Adsorbates from First Principles

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The development of efficient organic electronic devices depends substantially on the electronic coupling of the molecules at interfaces and on their arrangement at the nanometer length-scale. As an example, π-conjugated electronic systems maximize their coupling to a contact when they adsorb flat. An effective molecule-substrate interaction is mandatory for solar cells where excited electrons should be collected before recombination. Core electron spectroscopies are possibly the most suitable experimental technique to access fast electron transfer times, but introduce significant perturbation on the valence orbitals by the presence of core holes and bound excitons, further calling for theoretical analysis.

By first-principles simulations we investigate the resonant electron-transfer lifetime from the excited state of an organic adsorbate to a semiconductor surface, namely isonicotinic acid on rutile TiO2(110). The molecule-substrate interaction is described using density functional theory, while the effect of a truly semi-infinite substrate is taken into account by Green's function techniques. Excitonic effects due to the presence of core-excited atoms in the molecule are shown to be instrumental to understand the electron-transfer times measured using the so-called core-hole-clock technique. In particular, for the isonicotinic acid on TiO2(110), we find that the charge injection from the LUMO is quenched since this state lies within the substrate band gap. We compute the resonant charge-transfer times from LUMO+1 and LUMO+2, and systematically investigate the dependence of the elastic lifetimes of these states on the alignment among adsorbate and substrate states. [J. Phys. Chem. C, 2014, 118, 8775. DOI:10.1021/jp500520k]

A general method for functional optimization

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In particularly delicate systems, like liquid water, ab initio exchange and correlation functionals are simply not accurate enough for many practical applications. In these cases, fitting the functional to reference data is a sensible alternative to empirical interatomic potentials. However, a global optimization requires functional forms that depend on many parameters and the usual trial and error strategy becomes cumbersome and suboptimal. We present a general and powerful optimization scheme called data projection onto parameter space (DPPS). In an arbitrarily large parameter space, DPPS expands the vector of unknown parameters in vectors of known data. Poorly sampled subspaces are determined by the physically-motivated functional shape of ab initio functionals, using Bayes' theory to combine this prior information with reference energies and electron densities of monomers, clusters, and condensed phases of water.

Subsystem Density Functional Theory for Periodic Systems

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In recent years, the Frozen Density Embedding (FDE) formulation of subsystem DFT has been implemented in many quantum chemistry packages. However, none of the existing implementations are capable of tackling truly periodic systems, such as metal surfaces.

We fill this gap by introducing a new implementation of the Subsystem DFT method in the Quantum-Espresso package.

Highlights of our software include the capability of modeling an arbitrary number of subsystems, proper description of solid subsystems through Brillouin zone sampling, an accurate calculation of nuclear gradients to allow for geometry optimizations and molecular dynamics simulations, the constraining of charges and spin densities to allow simulation of ionic/radical subsystems.

We benchmark our method against molecular dynamics simulations of bulk liquids and solvated radicals, adsorption of molecules and molecular multi-layers on metals, as well as ionic organic crystals.

Future development will include the introduction of existing and the development of new non-local kinetic energy density functionals, to expand the domain of applicability of our subsystem DFT implementation.

Effects of anion doping on oxide-metal interface: a DFT study of MgO/Mo

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Abstract: Using density functional theory we have investigated how the work function of an oxide-metal system can be tuned by anion substitutional doping of the oxide. The model system we have considered is MgO supported over Mo (100), and nitrogen and fluorine are chosen as impurity atoms for doping of MgO. We have studied different MgO/Mo systems by varying both the concentration of the dopant atom in MgO and the position of the dopant atom with respect to the oxide-metal interface. Nitrogen acts as an acceptor, and fluorine acts as a donor type impurity when it replaces the oxygen atom in MgO. As expected, when the MgO is doped with the acceptor type impurity (N), the work function of the oxide-metal system is greater than the work function of the undoped system, and increases as a function of doping concentration. When MgO is doped with the donor type impurity (F), the work function of the system is expected to be lower than the work function in the undoped case. But interestingly we find that the work function behaves opposite to expectation for F-doped system. The trends in the work function in both systems are nicely explained using the trends shown by the dipole moments created in these N-doped and F-doped systems. To understand the contributing factors that lead to the dipole moments in these systems, we have separated out effects arising from the oxide-metal interface distance, the charge transfer between doped MgO and Mo, and the interface rumpling in the MgO layers.

REFERENCES:

(1) Prada, S.; Giordano, L.; Pacchioni, G. *J. Phys. Chem*. **2012**, 116, 5781-5786.
(2) Mammen, N.; Narasimhan, S.; Gironcoli, S. de. *J. Am. Chem. Soc*. **2011**, 133, 2801-2803.
(3) Saha, R. ; Revoju, S.; Hegde, V. I.; Waghmare, U.V.; Sundaresan, A.; Rao, C. N. R, *ChemPhysChem*, **2013**, 12, 2672-2677

Unravelling the origin of the E'_α and Ge(2) centers

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We present a first-principles investigation of Ge paramagnetic centers in vitreous silica and vitreous germania. An improved understanding of these paramagnetic defects is expected to have an impact in several scientific and technological fields ranging from silica-based optical fibers to future Ge-based microelectronic devices. EPR parameters are here obtained by exploiting the GIPAW method as implemented in the Quantum-Espresso package [1]. We generate and analyze a large number of Ge defect configurations that allow us to discuss structural models of the Ge-*E'* and Ge(2) centers in Ge-doped silica [2]. In particular, we provide evidence for an assignment of the Ge(2) center to Ge forward-oriented configurations, analogously to the E'_α center in silica [3], leading to an updated and unified picture of the defects in pure silica, germania and Ge-doped silica. Furthermore our work also addresses the Ge(2) precursor issue by showing that once a two-fold Ge atom (i.e a GLPC center) is ionized it can easily relax and give rise to a Ge forward-oriented configuration i.e. a Ge(2) center.

[1] P. Giannozzi *et al.*, *QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials* J.Phys.: Condens. Matter **21**, 395502 (2009).

[2] D. L. Griscom, *Trapped-electron centers in pure and doped glassy silica: A review and synthesis* J. Non-Cryst. Solids **357**, 1945 (2011).

[3] L. Giacomazzi, L. Martin-Samos, A. Boukenter, Y. Ouerdane, S. Girard, and N. Richard, *EPR parameters of E' centers in v-SiO2 from first-principles calculations* Phys. Rev. B **90,** 014108 (2014).

Local Reduced Density Matrix Functional Theory

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Local reduced density matrix functional theory (local RDMFT), is a theoretical scheme that incorporates static correlation effects in the Kohn-Sham equations, by abandoning the restriction of a single Slater determinant, through the use of fractional occupation numbers [1,2]. This allows the description of molecular dissociation without breaking spin symmetry. Additionally, our scheme provides a natural way to connect an energy eigenvalue spectrum to the approximate natural orbitals. This spectrum is found to represent accurately the ionization potentials of atoms, small molecules [1]. To demonstrate the computational efficiency of our method, we applied local RDMFT to molecular systems of relatively large size [2]. The results on the photoelectron spectrum of molecular systems and the relative stability of C20 isotopes are encouraging.

1. Nektarios N. Lathiotakis, Nicole Helbig, Angel Rubio, and Nikitas I. Gidopoulos, "Local reduced-density-matrix-functional theory: Incorporating static correlation effects in Kohn-Sham equations" Phys. Rev. A 90, 032511 (2014); http://dx.doi.org/10.1103/PhysRevA.90.032511

2. Nektarios N. Lathiotakis, Nicole Helbig, Angel Rubio, and Nikitas I. Gidopoulos, "Quasi-particle energy spectra in local reduced density matrix functional theory", J. Chem. Phys. 141, 164120 (2014); http://dx.doi.org/10.1063/1.489907

Magnetic Anisotropy Energy in Narrow Silicene Nanoribbons

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Magnetic anisotropy is the inhomogeneity of the magnetic properties when measured in different directions and is one key feature of the ferromagnetic nanostructures controlled by spin-orbit interaction [1, 2]. As an effect of the low-dimensionality of the ribbons, the observed magnetic properties are mainly produced by the edge-localized states and they are different from those observed in the bulk [3].

We report the magnetic anisotropy arising from the edges of silicene narrow ribbons. An All-electron full-potential linearized augmented-plane wave (FP-LAPW) code within density functional theory was applied. In particular we study how changes the total energy of the system as a function of the direction of its magnetic moment.

The main result of our work is the strong dependence on the direction the magnetic moment –and therefore on the quantum numbers J and S– of the system total energy, where we have found changes with the angle in the total energy of the system in the order of a few meV.

[1] Chikazumi, S. Physics of Ferromagnetism 2e; Oxford University Press, 2009.

[2] Hernando, A.; Crespo, P.; García, M.; Pinel, E. F.; de La Venta, J.; Fernández, A.; Penadés, S. Physical Review B 2006, 74, 052403.

[3] Rusponi, S.; Cren, T.; Weiss, N.; Epple, M.; Buluschek, P.; Claude, L.; Brune, H. Nature Materials 2003, 2, 546–551.

Speeding up linear-response DFT calculations with optimally reduced plane-wave basis sets

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State-of-the-art approaches to linear response in DFT rely on numerical methods that allow one to avoid computing unoccupied Kohn-Sham (KS) orbitals altogether [1, 2]. When using plane-wave (PW) basis sets, the price to be paid is the necessity to handle ill-conditioned operators whose representation may require a very large number of PW's. When using iterative techniques to compute linear-response functions, such as, e.g., in the Liouville-Lanczos approach within TDDFT to optical absorption spectroscopy of finite systems [3, 4] or electron energy-loss and inelastic X-ray scattering spectroscopies of periodic solids [5, 6], this results in a large numerical cost to perform each individual iteration and in a number of iterations that increases with the operator condition number. In order to mitigate these problems, we propose to tackle response KS orbitals, using a mixed representation made of a very small number of unoccupied KS orbitals and a small number of orthogonalized PW's. We have implemented our approach in the development version of the Quantum ESPRESSO package [7]. In this poster we describe this approach and demonstrate it with a few test case calculations of optical absorption spectra in small molecules.

[1] S. Baroni, S. de Gironcoli, A. Dal Corso, and P. Giannozzi, *Rev. Mod. Phys.* **73**, 515 (2001).

[2] S. Baroni and R. Gebauer, Chapter 19 in M.A.L. Marques, N.T. Maitra, F.M.S. Nogueira, E.K.U. Gross, and A. Rubio "Fundamentals of Time-Dependent Density Functional Theory", vol. 837, Springer-Verlag, Berlin (2012).

[3] D. Rocca, R. Gebauer, Y. Saad, and S. Baroni, *J. Chem. Phys.* **128**, 154105 (2008).

[4] X. Ge, S.J. Binnie, D. Rocca, R. Gebauer, and S. Baroni, *Comp. Phys. Comm.* **185**, 2080 (2014).

[5] I. Timrov, N. Vast, R. Gebauer, and S. Baroni, *Phys. Rev.* **B 88**, 064301 (2013).

[6] I. Timrov, PhD thesis, Ecole Polytechnique, France (2013) https://pastel.archives-ouvertes.fr/pastel-00823758.

[7] P. Giannozzi, S. Baroni et al., *J. Phys. Condens. Matter* **21**, 395502 (2009) http://www.quantum-espresso.org.

Ferromagnetic iron as a topological metal

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Topological metals are a recently-proposed phase characterized by the presence of disconnected Fermi surface (FS) sheets with nonzero Chern indices[1]. This requires the presence of spin-orbit coupling, and that either spatial inversion (P) or time-reversal (T) symmetry is broken. Under these conditions most accidental degeneracies are lifted, except for isolated band touchings (and possibly a few line nodes on symmetry planes). The isolated band-touching points (Weyl nodes) cannot be easily removed, and act as monopoles of Berry curvature, which in turn gives rise to the intrinsic anomalous Hall conductivity (AHC). The Chern number of each individual FS sheet is given by the net enclosed topological charge. Here we show that bcc iron is a topological metal, and analyze the implications for the AHC. First we carry out a systematic search for band touchings in the bandstructure, using first-principles calculations. We find numerous degeneracies, mostly Weyl points (linear crossings) carrying charge ±1, but also several double-Weyl nodes (quadratic band touchings) with charge ±2. Nevertheless, most FS sheets are topologically trivial, with zero Chern index. The reason is that they surround P-invariant points in the BZ, so that the enclosed Weyl nodes come in pairs of equal and opposite charge. The exceptions are two small electron pockets on the [001] ΓH line parallel to the magnetization. Each of them encloses a single Weyl node, leading to Chern indices of ±1. The contribution of these two pockets to the AHC is given, modulo a G vector, by their reciprocal-space separation, as in a magnetic Weyl semimetal. In order to resolve the quantum of indeterminacy **G** we plot isocontours of the Berry phase calculated along [010] strings of k-points, which carry the same topological information as Fermi arcs in the (010) surface bandstructure.

[1] F. D. M. Haldane, arXiv:1401.0529 (2014).

High performance electronic structure engineering with hybrid DFT and GW

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We present methodological and algorithm developments for the calculation of the electronic structure of large systems with hybrid density functional theory (sc-hybrid) and many body perturbation theory (GW). In particular, we will discuss sc-hybrid functionals derived within a generalized Kohn-Sham scheme, where the fraction of exact exchange is determined self-consistently using dielectric susceptibilities [1]. We will also discuss the parallel efficiency of a recently proposed GW technique that does not require the computation of virtual orbitals, and its application to systems with thousands of electrons, including semiconductor nanoparticles, solid/liquid interfaces and defective materials [2].

[1] J.H. Skone, M. Govoni and G. Galli, *Self-consistent hybrid functional for condensed systems*, Phys Rev B 89, 195112 (2014)
[2] M. Govoni and G. Galli, *Large scale GW calculations*, submitted.

This work was supported by ARL, grant number W911NF-12-2-0023.

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

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Semiconductor-based thin-films have applications in microelectronics, from transistors to nano-capacitors [1]. Many of their properties depend on phenomena at multiple length scales, but their complexity makes it difficult to obtain a detailed understanding of their behavior from experiment alone.

First-principles simulations based on density-functional theory (DFT) are invaluable for providing insight into materials' properties including for the study of thin films. In particular, hybrid Wannier functions (WFs), fully extended in the surface plane, but localized along the direction normal to the surface, have been successfully used to explore the properties of systems layered along a given direction [2]. The large length scales associated with structures and processes in more realistic surfaces, however, are beyond the scope of such calculations, because they rely on first performing a traditional cubic-scaling DFT calculation.

To overcome this limitation we extend the concept of hybrid WFs to nonorthogonal orbitals that are directly optimized *in situ* in the electronic structure calculation. We show that this method, implemented in the ONETEP linear scaling DFT code [3], enables the study of large-scale surfaces and interfaces with plane-wave accuracy but at reduced computational expense.

References:

[1] Fortunato et al., Advanced Materials, 24, 22 (2012).

[2] Giustino et al., Phys. Rev. Lett. 91, 267601 (2003).

[3] C.-K. Skylaris et al., J. Chem. Phys. 122, 084119 (2005).

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

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Highly Oriented Pyrolitic Graphite (HOPG) can be described as stacked graphene layers. Due the weak van der Waals interaction between the layers, topmost layer of HOPG can be rotated or shifted by chemical or mechanical means. With rotation of the topmost layer, super periodic structures called as moiré patterns are formed. In this work, moiré patterns on HOPG surfaces due to dislocated graphene layers were studied. A simple geometric investigation of the atomic structure of the moiré patterns revealed that different atomic moiré periodicities result in similar geometric moiré periods, which bring forth the importance of information on the real atomic structure of each moiré pattern observed in STM images. Our calculations showed that the band structure of moiré patterns even though exhibits the fingerprints of those of twisted bilayer graphene system, like the preserved Dirac cone at the K point of moiré Brillouin zone, it has several new emerging features like van Hove singularities and linear or flat bands depending on the moiré periodicity. Our results show that most of the moiré patterns observed on graphene/HOPG system do not have a purely electronic or structural origin, but both. Moreover, our results show that van Hove singularities in these systems with different twist angles have different origins in their respective band structure.

Valence Band Structure of Square Quantum Well Under Stress

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Valence band structure with spin-orbit (SO) coupling of GaAs/$Ga_{1-x}Al_xAs$ square quantum well (SQW) under stress along the [100], [001], [110], [111] directions and hydrostatic stress by a calculation procedure based on a finite element method (FEM) is investigated using the multiband effective mass theory ($\vec{k}.\vec{p}$ method). The validity of the method is confirmed with the results of Ahn and Chuang [1] who calculated valence band structure, using axial approximation for Luttinger-Kohn Hamiltonian and finite difference method. Our results demonstrate that SO coupling and stress have significant effects on the valence band structure.

Key words: Finite Element Method; Valence subband structure; multiband effective mass theory.

Electronic and Optic Properties of Corrugated Quantum Wells

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In this study, the effects of stress, electric field and well width on the electronic band structure and the optic properties of a single corrugated $Ga_{1-x}Al_xAs/Ga_{1-y}Al_yAs/Ga_{1-x}Al_xAs$ quantum well is investigated with effective mass approximation by combining the finite element method. According to the findings, the electronic and optic properties of a single corrugated $Ga_{1-x}Al_xAs/Ga_{1-y}Al_yAs/Ga_{1-x}Al_xAs$ quantum well system can be adjusted for the changes in σ parameter, electric field, well width and stress.

Key words: Corrugated quantum well, finite element method, intersubband absorption, stress, electic field.

Electronic structure of substitutionally disordered systems: orbital-based CPA within a pseudopotential approach

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The study of the electronic structure of substitutionally disordered systems (e.g. doped compounds) via density functional-based methods is a challenge. A common approach based on supercells is limited to special impurity concentrations and is numerically expensive. Effective medium theories are more promising to deal with arbitrary impurity concentrations where interesting physics can emerge. One of these methods, the coherent potential approximation (CPA), has already been successfully applied in the KKR framework. Blackman Esterling and Berk (BEB) have developed an extension of the CPA which allows to handle also off-diagonal disorder on the level of the hopping terms [1].

In this work we discuss the development of a charge self-consistent BEB-CPA within a pseudopotential approach. We project the Kohn-Sham orbitals self-consistently obtained in a mixed-basis representation onto a localized nonorthogonal LCAO basis. Based on earlier work for an all-electron method [2] we then set up the BEB-CPA within this LCAO-pseudopotential framework. From a self-consistent CPA medium we calculate the electronic density to improve the Hamiltonian for a new BEB-CPA calculation. We present model studies to numerically verify the BEB-CPA for a tight-binding binary alloy Hamiltonian against exact diagonalization. Further we present first results of treating real materials with our code.

[1] J.A. Blackman et al., Phys. Rev. B 4, 2412 (1971)

[2] K. Koerpenik et al. Phys. Rev. B 55, 5729 (1997)

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

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Despite the fact that first-principles density-functional-theory modelling has objectively entered the industrial world, the essential requirement to access material properties at operating conditions (finite temperature) in large systems remains a challenge.

Very recently second-principles effective methods have been developed that (i) capture the main interatomic and electronic interactions of materials in a totally generic and mathematically simple form, (ii) rely on parameters automatically computed from accurate first-principles calculations, and (iii) allow for meso-scale statistical simulations at operating conditions keeping first-principles accuracy and predictive power.

While not so restricted in size, second-principles simulations are usually focused on either electronic or lattice properties. However, both degrees of freedom are important in many physical problems and should be treated on the same footing.

We present here an approach that accurately reproduces *ab-initio* results for systems including reasonably localized electrons like complex oxides or semiconductors. This scheme combines a reliable model potential for the lattice [1] with a modified self-consistent tight-binding method including both long-range electron-electron and short-range strong correlation interactions. Only the active electrons and holes (those that play a relevant role in the determination of the physical magnitude of interest) are retained in the description of the electronic properties. The interaction of lattice and electron includes both electrostatics and short-range terms allowing the description of a wide range of phenomena. Combined with an efficient Lanczos-based diagonalization, our method provides a systematically improvable scheme to simulate systems including tens of thousands of atoms under experimental conditions.

Here we will present examples of systems including relatively localized electrons, and where the electron-lattice interaction is fundamental, such as the formation of polarons in bulk $SrTiO_3$ and the metallicity at the $LaAlO_3/SrTiO_3$ interface.

[1] J. Wojdeł, P. Hermet, M. P. Ljungberg, Ph. Ghosez, and J. Íñiguez, J. Phys.: Condens. Matter **25**, 305401 (2013).

Thermoelectricity: Coupling transport equations and *ab initio* calculation

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Keywords: thermoelectricity, electron-phonon coupling, Boltzmann transport equation

The search for materials that can produce electrical power from a temperature gradient - the Seebeck effect-, has gained significant interest in recent years. Indeed thermoelectric materials have proved to be viable solutions for the remote generation of electrical power in satellites [1]. The reverse (Peltier) effect allows to cool down electronic components in devices through a cold pole obtained with an electrical current passing through a junction of two conductors. The efficiency of a thermoelectric material is characterized by the figure of merit ZT [2], which is proportional to the electrical conductivity (σ) and to the square of the Seebeck coefficient (Q), and inversely proportional to the thermal conductivity (κ).

Improving the efficiency of thermoelectric devices requires an understanding of the mechanisms that control electronic transport. In particular, in semiconductors, the Seebeck coefficient increases drastically as the temperature decreases [3-4]. This is known as the phonon-drag effect: phonons carrying a thermal current tend to drag the electrons with them from the hot side to the cold side of the sample. The phonon-drag effect leads to the improvement of the figure of merit ZT. However, the phonon-drag effect cannot be described in the framework of usual Boltzmann transport equations (BTE) [5-6]. In the first part of this presentation, we will present the approach to study the phonon-drag effect in materials [7].

At the same time, solving the transport equation for the electrons requires the knowledge of the electronic structure and of the carrier interactions (electron scattering on impurities and electron-phonon scattering). A good description of these physical mechanisms is achieved by parameter-free calculation in the framework of density functional theory (DFT) [8]. In a second part of the presentation, we will describe an approach based on the coupling of the Boltzmann transport equation with DFT calculations of the electronic structure and the electron-phonon coupling [6-7]. It has been successfully applied to the determination of the thermoelectric properties of bulk silicon [9]. This approach has the advantage of reducing the number of adjustable or *ad hoc* parameters in simulation of transport properties and thus leads to a better understanding of the underlying physical laws, as shown in Ref. [8-9].

References

[1] A. Bulusu, D.G. Walker, Superlattices and Microstructures 44 (2008).

[2] Ali Shakouri, Annu. Rev. Mater. Res. 2011. 41:399-431.

[3] Geballe and Hull, Phys. Rev. 98, 940 (1955).

[4] Conyers Herring, Phys. Rev. 96, 1163 (1953).

[5] M. Lundstrom, Fundamentals of Carrier Transport, Cambridge University Press, 2009.

[6] *"Simulation of transport in nanodevices", Ed.* ***Philippe DOLLFUS*** *and François TRIOZON, 2 volumes. Chapitre 1 du volume 1 : Electrons, phonons, and their coupling within the density functional theory,* ***Nathalie VAST, Jelena SJAKSTE, Gaston KANÉ*** and Virginie TRINITÉ, accepted (2014).

[7] *First-principles calculations of electron-phonon scattering,* J. Sjakste, I. Timrov, P. Gava, N. Mingo, N. Vast , *Annual Reviews of Heat Transfer*, Begell House (in press, 2014*).*
DOI: 10.1615/AnnualRevHeatTransfer.2014007320

[8] Jelena Sjakste, Nathalie Vast and Valeriy Tyuterev, Phys. Rev. Lett. 99, 236405 (2007).

[9] Z. Wang, S. Wang, S. Obukhov, N. Vast, J. Sjakste, V. Tyuterev, and N. Mingo, Phys. Rev. B. 83, 205208 (2011).

Interplay between defects and stacking at the SiC/SiO$_2$ interface

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Silicon Carbide is a wide band-gap semiconductor material that can be used for high temperature and power electronic devices, such as field effect transistors. These are conditions under which the traditionally used Silicon fails.

Like Si, the native oxide of SiC is SiO$_2$, but its use in practical devices has been hampered by the low channel mobility of the SiC/SiO$_2$ interface. This has been attributed to defects in the interfacial region, several types of which have been identified in previous studies [1][2].

In this work we performed electronic structure calculations using the RSPACE [3] code to investigate the effect of SiC stacking on the electronic properties of the SiC/SiO$_2$ interface, both in the presence and absence of defects. Measures such as the energies and Local Density of States (LDOS) of these structures were used as a means of comparison.

The interface was modelled using 4H-SiC and β-tridymite SiO$_2$, allowing for 4 possible variations of the clean interface, based on the SiC stacking and the relative positions of the SiC and SiO$_2$. Of these, the SiC stacking has the more significant effect.

Defects, such as excess C or O atoms, were then introduced into the interfacial region. Expanding on previous studies, several positions were investigated for each defect, in addition to the different SiC stackings.

We have found that the effect of defects on the interface LDOS varies with SiC stacking. In addition, some changes occur regardless of defect type. By comparison, defect position usually has relatively little effect.

[1] P. Deak *et al.*, *J. Phys. D: Appl. Phys.* **40**, 6242–6253 (2007)
[2] A. Gavrikov *et al.*, *J. Appl. Phys.* **104**, 093508 (2008)
[3] Hirose K, Ono T, Fujimoto Y, Tsukamoto S: *First-Principles Calculations in Real-Space Formalism*. London: Imperial College Press; 2005.

A General Purpose Massively Parallel *Ab Initio* Molecular Dynamics Implementation With A Linear Scaling Exact Exchange Algorithm

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Density functionals that account for exact exchange (*Exx*) have been successful in describing many physical quantities including the strength of hydrogen bonds in various ice phases [1], defect energies of semiconductors [2], and the structure of ambient liquid water [3]. However, the cubic scaling in conventional reciprocal space based *Exx* algorithms makes the application of hybrid density functionals to large scale *ab initio* molecular dynamics (AIMD) simulations computationally very demanding. In this work, we have implemented a linear scaling *Exx* algorithm [4] as a general-purpose module in the Quantum ESPRESSO (QE) package. To achieve realistic simulation wall times, this implementation efficiently incorporates the OpenMP and MPI parallelization paradigms to utilize 10,000-100,000 cores. We demonstrate the performance of this implementation using several condensed-phase systems including a series of liquid water samples with different supercell sizes that contain up to a few thousands of atoms.

[1] B. Santra, J. Klimeš, D. Alfè, A. Tkatchenko, B. Slater, A. Michaelides, R. Car, and M. Scheffler, Phys. Rev. Lett. **107**, 185701 (2011).

[2] C. Di Valentin, G. Pacchioni, and A. Selloni, Phys. Rev. Lett. **97**, 166803 (2006).

[3] R. A. DiStasio Jr., B. Santra, Z. Li, X. Wu, and R. Car, J. Chem. Phys. **141**, 084502 (2014).

[4] X. Wu, A. Selloni, and R. Car, Phys. Rev. B **79**, 085102 (2009).

We graciously acknowledge support from the DOE Grant DE-SC0008626.

First-Principles Study Of Oxide Superlattices

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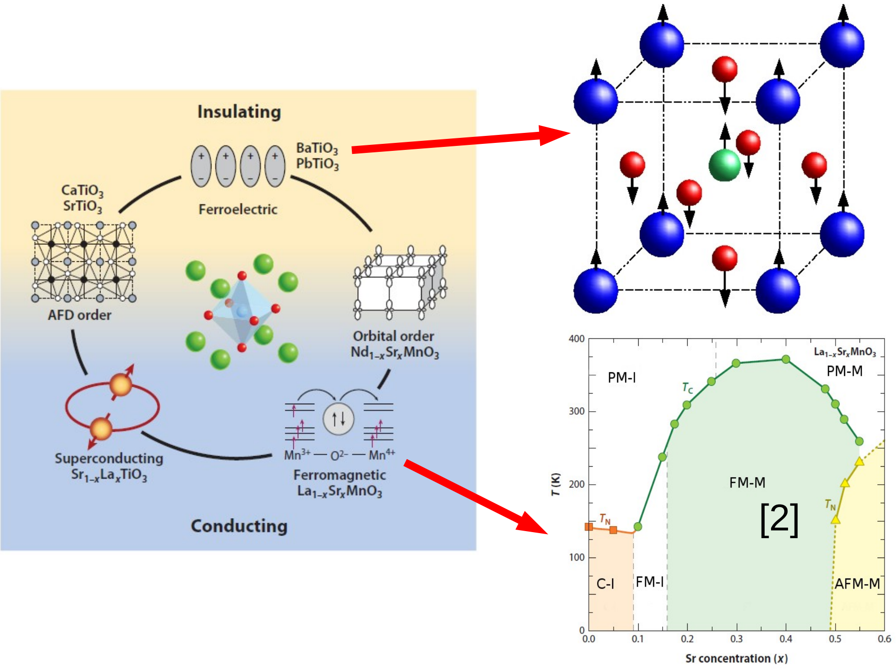
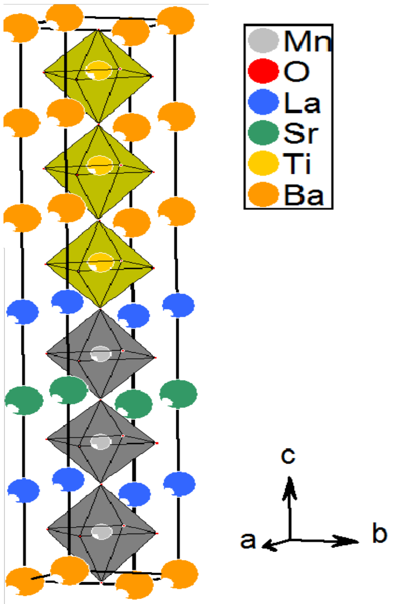
Perovskite oxides form an important family of materials, exhibiting a wide variety of functional properties exploited in various devices. These oxides can also be combined in heterostructures. Creating articial superlattices (SL) of perovskite oxides gives not only the possibility to combine their intrinsic properties but also to induce totally new phenomena at their interfaces. We investigate theoretically the properties of manganites in which orbital ordering can be observed. We consider three layers $La_{2/3}A_{1/3}MnO_3$ (A = Sr or Ba) (LAMO = LSMO or LBMO) and combining them with three layers of ferroelectric $BaTiO_3$ (BTO) or six layers of paraelectric BaO (BO) grown on a $SrTiO_3$ (STO) substrate. This work is motivated by the recent discovery of a large increase of the Curie temperature (T_c = 650 K) in BTO/LSMO superlattices compared to the bulk LSMO (T_c =370 K) thanks to the mechanism arising through orbital ordering [1]. However, the role of ferroelectic block was neglected, as the antiferrodistortive motions (AFD) in LSMO or the interface between the two materials. We aim to study the potential role of AFD oxygen rotations of LAMO, to clarify the role of spontaneous polarızation of BTO, to study the interface effects.





1] A. Sadoc et al, PRL 104 046804 (2010)
[2] P. Zubko et al, Annu. Rev. Condens. Matter Phys. 2 141 (2011)

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

Title: Conversion of Toxic H_2S to Green Fuel H_2 with 2D-$ZnO_{1-x}N_y$

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Abstract: (250 words)

We present a thorough analysis of molecular adsorption of a toxic gas, H_2S, on pristine, defective and N-substituted 2D-ZnO using first-principles density functional theory simulations with parametrized form of van der Waals (vdW) interaction. We find that the binding of H_2S with pristine 2D-ZnO is relatively weaker (adsorption energy $E_A = -29$ to -36 $kJmol^{-1}$) as it is mainly through vdW interaction. However, substitution of nitrogen for oxygen in 2D-ZnO leads to a drastic increase in the adsorption energy ($E_A = -152$ $kJmol^{-1}$) resulting in dissociation of H_2S molecule. This originates fundamentally from a strong covalent bonding interaction between an unpaired electron in the p-orbital of nitrogen with an electron in s-orbital of H. While O-vacancy in 2D-ZnO has little effect on its interaction with H_2S at lower coverages, a strong interaction at higher coverages leads to splitting of H_2S and formation of H_2 molecule. Our work shows that 2D-ZnO has the potential to facilitate capture of toxic H_2S from environment and its conversion to hydrogen, a green source of energy.

Metal-Insulator Transition and Lattice Instability of Paramagnetic V_2O_3

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We determine the electronic structure and phase stability of paramagnetic V_2O_3 at the Mott-Hubbard metal-insulator phase transition, by employing a combination of *ab initio* methods for calculating band structures with dynamical mean-field theory [1]. To explore structural transformations as a function of pressure, we use the experimentally determined atomic positions for the metallic and insulating phases, respectively, and calculate the total energy as a function of volume. We find that the structural stability depends very sensitively on changes of the lattice volume. The structural transformation associated with the metal-insulator transition is found to occur upon a slight expansion of the lattice volume by $\sim$ 1.5 %, in agreement with experiment. Our results show that the structural change precedes the metal-insulator transition, implying a complex interplay between electronic and lattice degrees of freedom at the transition. Electronic correlations and full charge self-consistency are found to be crucial for a correct description of the properties of V_2O_3.

[1] I. Leonov, V. I. Anisimov, and D. Vollhardt, arXiv:1410.5399