The Abdus Salam
International Centre for Theoretical Physics

POSTER SESSION I

THURSDAY 13 JANUARY 2011

In alphabetical order of presenting author (underlined)

Beyond DFT: Taking into account charging energy and semiclassic electron-phonon coupling
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Ultrasoft pseudopotentials and projector augmented-wave data-sets: application to diatomic molecules
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Fully self-consistent LDA+DMFT Calculations: A plane wave and projector augmented wave implementation and application to the study of Cerium compounds.
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First-principles study (GW+PAW) on new oxynitride phosphors for white LED
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Regarding the Structural Phase Transitions and sp-d Hybridization in Cubic Calcium
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Local Density Approximation plus Gutzwiller Method, a Siesta implementation
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Energetics and metastability of the silicon vacancy in cubic SiC
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Influence of biaxial strain on spinodal decomposition in magnetic semiconductor alloys
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Atomic and electronic structure of Co2CrAl/NaNbO3/Co2CrAl magnetic tunnel junctions
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Solvation and thermal effects on the optical properties of natural dyes: a case study on the flavylium cyanin
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Long-wavelength properties of metallic systems studied by ab initio methods
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Dynamical response function in Sodium and Aluminum from Time-Dependent Density-Functional Theory
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First principles EPR spectra of transition metal complexes
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The projector augmented–wave method: application to relativistic spin–density functional theory
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Analysis of thermodynamic, thermoelectric and magnetic properties of FeSb2 in the framework of density functional theory
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Ab-initio investigation of lattice dynamics in substitutional disordered alloys
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Magnetism & magnetic anisotropies of small structures containing 5d atoms
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Electronic response in Koopmans corrected functionals: polarizabilities and hyperpolarizabilities of linear chains
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First-principles study of the magnetic phase diagram of LaOx−1FxFeAs
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Electronic circular dichroism for Guanine-Cytosine base pairs in Watson-Crick and Hoogsteen configuration
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Many Body Perturbation Theory simulations of the electronic properties of large DNA models.
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The interactions of nitrogen dioxide with graphene and with Rh clusters stabilized by graphene
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Role of the Pressure in the Elastic Properties of Ce

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Local Field Effects in Silicon Nanocrystals

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

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Elasticity and Conductance interplay in model molecules

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

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Formalism for GW calculations without empty states in a localized basis

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Ab initio investigation of topological insulators

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Linear Response TDDFT in CASTEP: An HPC Implementation
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Total Energy Formalism for Charged Nanocapacitors: Orbital Partition Approach
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Electron-electron interactions in superconducting Lithium under pressure
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Resolving Controversies on the Multiple Conductance Peaks in Single- Molecule Junction Experiments by Multiscale Simulations
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Expanded radialenes carbon nanotubes: electronic and elastic properties
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Determination of NMR chemical shifts for cholesterol crystals from first-principles
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Pressure induced unified study of strongly correlated ErSb
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Direct calculation of the one particle Green's function: an alternative to the self-energy
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Electronic correlations at the α-γ structural phase transition in paramagnetic iron

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High-pressure Raman spectra of TiO2

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Magnetism in FeMn Nanostructures

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Study of the relaxation of the Aluminum cluster in the self-compressed inhomogeneous stabilized jellium model

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RVB states in graphene and other carbon compounds

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Spin and valley susceptibility in wide AlAs quantum wells

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A self-consistent, first-principles method for complex disordered materials

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MICROMAGNETIC SIMULATIONS OF FIELD INDUCED DOMAIN WALL MOTION IN Fe20Ni80/Cu/Co SPIN VALVE

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First-principles Study of P3HT/ZnO Hybrid Organic-Inorganic Photovoltaic Interface

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p Magnetism in CaC: First principle study

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Stability of domain boundaries on the Ge-covered 5×5-reconstructed Si(111) surface

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First-principles study of O1s core-level shifts at dye-sensitised solar cell interfaces

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Nonlinear Elasticity of Graphene and Other Hexagonal Carbon Allotropes

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Ab-initio calculations of absorption spectra of nanowires by solving the Bethe-Salpeter Equation

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Dispersion interactions in room-temperature ionic liquids: Results from a non-empirical density functional

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Edge effects in graphene nanoislands on Co(0001)

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Surface-induced magnetism in C-doped SnO2: First-principles study

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Monte Carlo modeling of structural properties in compressed 2D Wigner crystals

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Surface-induced atomic and electronic properties of unpassivated GaAs Nanowires

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Electronic properties of crystal and amorphous phases of SiO2: disorder effects within and beyond Density Functional Theory

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DFT and Beyond - Climbing Jacob’s Ladder

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Polynitrogen confined to C60 Cage: A novel energetic Material

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A unified pseudopotential approach to superconducting state parameters of Mg, B and MgB2

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Electronic structure of hydrogenated diamond surfaces: The role of temperature on surface reconstruction
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The nonempirical calculations of the lattice dynamics of the oxyfluoride Rb2KTiOF5
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Pseudo-electromagnetism in graphene
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PAW method in localized-basis-set SIESTA code: first stage of development
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A simulated reflectivity experiment: theoretical optical spectrum of strained-lattice bulk SrTiO3
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Ab initio study of electronic properties of bismuth
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Numerical simulation of four-probe resistance measurements of nanoscale materials
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Characterization of point defects in UO2 by positron annihilation spectroscopy: a first-principles study
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Electron-phonon coupling in semiconducting nanostructures
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The absorption of diamondoids from time-dependent density functional calculations
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Ab initio prediction of giant magnetoelectric effects driven by structural softness
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A DFT/TDDFT study of di-zinc pyrazinoporphyrazine-phthalocyanine complexes with different peripheral substituents as potential sensitizers in a DSC
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A theoretical study of the effect of the bridge (=CH-, =N-, -O-, -S-) connecting di-Zinc pyrazinoporphyrazine-phthalocyanine complexes
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Optical properties and aromaticity of meso substituted porphyrins
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The role of van der Waals forces in semiconductor solids
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Beyond DFT: Taking into account charging energy and semiclassic electron-phonon coupling.

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Although DFT, in LDA and GGA approximation is an state-of-the-art technique for a full variety of systems such as molecule adsorption, carbon nanotubes and bulk structures [1], it presents well-known shortcomings on systems where correlation or electron-phonon interaction are important; such as organic molecular conductors , metal/organic semiconductors interfaces [2], or chlorophyl or chromophore dynamics.
In this work we present on one hand, a way to estimate the charging energy for the case of metal/organic interfaces using a simple model that allows us to correct the DFT gap [2]. On the other hand, in order to deal semiclassically the electron-phonon interaction, beyond DFT a molecular dynamics with electronic transition method is presented [4]. All these corrections has been included in the first principle code FIREBALL [3].

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Ultrasoft pseudopotentials and projector augmented-wave data-sets: application to diatomic molecules

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We test several ultra-soft pseudopotentials (US-PPs) and projector-augmented wave (PAW) data-sets, calculating the bond lengths, the atomization energies and the frequencies of the vibrational stretch modes of several diatomic molecules. The same parameters are used to construct both the US-PPs and the PAW data-sets using the local density approximation (LDA) or the Perdew, Burke and Ernzerhof (PBE) generalized gradient approximation. The dimers H_2, O_2, F_2, Al_2, Si_2, P_2, S_2 and Cl_2 and several combinations of B, C, N, O, F, Al, Si, P, S, Cl, Fe, Ni, with H, C, N, and O are considered and the convergence of the calculated quantities with the size of the plane waves basis set is studied in detail. We found that US pseudopotentials and the PAW data sets constructed with the same parameters, provide almost equivalent results for both the bond lengths and the vibrational stretch frequencies. Instead, in some cases the PAW method gives atomization energies which are closer to the all-electron values than the US-PPs method. The calculated geometries and vibrational frequencies are compared with the results obtained by localized basis sets present in the literature and it is found that the agreement is quite good, expecially when extended localized basis sets (such as the aug-cc-pVTZ) are used.

Fully self-consistent LDA+DMFT Calculations: A plane wave and projector augmented wave implementation and application to the study of Cerium compounds.

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The combination of Density Functional Theory (DFT) in the Local Density Approximation (LDA) and Dynamical Mean Field Theory (DMFT) has been used in the past years to understand properties of strongly correlated electron systems. We present here a implementation of LDA+DMFT, using projected local orbitals, which includes full self-consistency on the electronic density, within the Projector Augmented Wave (PAW) framework. This thus opens the way to accurate calculations including relaxation with the simplicity of a plane wave code and the all-electron precision. We compute spectral function and total energy for this implementation and apply it to cerium compounds.

First-principles study (GW+PAW) on new oxynitride phosphors for white LED

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After the original incandescence lamp, after the invasion of compact fluorescent lamps, white-LEDs will be one of the major actor involved in the future generations of eco-friendly light sources. However, with the exception of incandescence lamp, all types of white light source require the use of phosphors. For novel types of white LEDs, an optimal combination of two green- and red-emitting phosphors absorbing partly the blue light from the InGaN LED is mandatory to obtain a white light source by post recombination of the light.

We have theoretically studied two oxynitride phosphors, one of which is an efficient green phosphor $Ba_3Si_6O_{12}N_2$:Eu developed at the Mitsubishi Chemical Group Science and Technology Research Center, and the other is a bluish-green phosphor $Ba_3Si_6O_9N_4$:Eu that exhibits little luminescence at room temperature. Our first-principles results rely on many body perturbation approach (GW+PAW) applied to the two hosts for Europium dopants : $Ba_3Si_6O_{12}N_2$ and $Ba_3Si_6O_9N_4$. The calculation shows a slightly narrower energy gap for $Ba_3Si_6O_9N_4$, that is 0.33 eV. Yet such a result provides precious keys to understand the thermal quenching mechanism, by comparing materials with a similar chemical composition, but different thermal behaviour. As a next step a deeper analysis with Eu-doped models will shed new light onto the relationship between emission/excitation colors from the Europium luminescent centers, and the properties of their complex ligands (dielectric properties, coordination).

Regarding the Structural Phase Transitions and sp-d Hybridization in Cubic Calcium

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Ultrasoft pseudopotential (U-PP) is used for core electrons to solve Kohn-Sham density functional within the generalized gradient approximation due to Perdew-Burke-Ernzerchhof (PBE) parameterization scheme. Total energies and thereby enthalpies are calculated for FCC, BCC and SC phases using the Quantum–Espresso (PWscf) package, which predict only correct pressure induced structural phase sequence, i.e., FCC→BCC in elemental calcium. However, BCC→SC transition is not observed upto the pressure of 60 GPa. Also, to examine FCC→BCC martensite structural phase transition (SPT) at finite temperatures, we have employed the concept of mean-field potential (MFP) approach in conjunction with the *evanescent* form of the local pseudopotential. The MFP approach is considered to be the good working proxy [e.g., see Philo. Mag. **90**, 1599-1622 (2010)] to account for the anharmonicity in lattice dynamics and thereby in different thermodynamic properties, which is otherwise difficult to compute due to its many-body nature. Parameters of the local potential used are optimized for cohesive properties at ambient condition with the U-PP based PWscf results. This also gives only correct FCC→BCC transition at 20 GPa in agreement with the experiment. However, high-T FCC→BCC and high-P BCC→SC phase changes can be identified only after including the effect of sp-d hybridization. In the present study, we have used 3d–hydrogenic wave function to obtain this overlap potential. Incorporation of so obtained parametric hybridization potential not only shows BCC→SC transition at 32.75 GPa, but also stabilize BCC phase at higher temperatures in accordance with the experiment. For example, the figure examplifies that the Gibbs free energy for BCC phase with hybridization lowers below the FCC phase at T = 738 K, while the same but without considering the overlap effect remains too high upto the melting temperature. In its simplest explanation, present study therefore confirms that the FCC→BCC transition at lower pressures is governed solely by the Madelung contribution, while BCC→SC transition at further compressions requires inclusion of hybridization effect. We also conclude that at finite temperatures hybridization effect only is suffice to mimic the phase transition, and d-band filling is certainly not required. Thus, calcium in high-T regime behaves like empty-d-band metal.

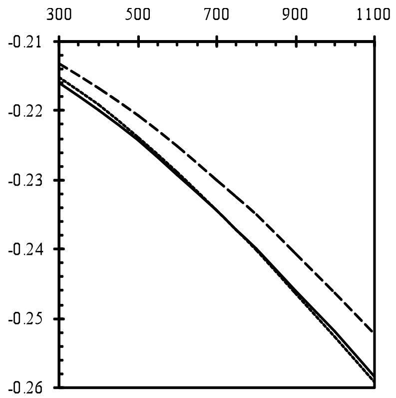

Fig.: Gibbs free energy as a function of temperature for cubic phases: FCC phase (solid line), BCC phase with (dotted line) and without (long-dashed line) hybridization effect.

Local Density Approximation plus Gutzwiller Method, a Siesta implementation

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Gutzwiller variational method, as used in Monte Carlo simulations on lattice models, provides a way to optimize an electronic wavefunction by changing the double occupation probability of single sites. While acting only on a local Hilbert space, the Gutzwiller projector has the effect of renormalizing the mass of quasiparticles, and therefore the effective hopping between sites. In our work we try to apply the Gutzwiller variational approach to realistic systems. This goal is achieved thanks to Density Functional Theory, where the Local Density Approximation is improved by applying the Gutzwiller projector to a selected set of atomic orbitals. As a result, the Kohn Sham quasiparticle is substituted by a Gutzwiller quasiparticle with a renormalized mass and a variationally improved Hartree and Exchange-Correlation functional. Our approach is theoretically consistent with the Levy-Lieb formulation of DFT. We decided to adapt the Siesta package for our aims, since it is a flexible simulation code using an atomic basis set which allows for a natural parametrization of the Gutzwiller projector.

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Energetics and metastability of the silicon vacancy in cubic SiC Fabien Bruneval and Guido Roma CEA, DEN, Service de Recherches de M\'etallurgie Physique, F-91191 Gif-sur-Yvette, France The silicon vacancy is a prominent intrinsic defect of cubic SiC (3C-SiC) to which much effort has been devoted so far, experimentally and theoretically. We calculate its properties using the state-of-art GW approximation that does not suffer from the band gap problem. The obtained formation and transition energies deviate significantly from the usual density functional theory evaluations and now compare favorably with experiment. A new assignment for the main line of photoluminescence is then proposed. We further perform GW calculations for the saddle point of reaction paths. The resulting barrier energies explain the thermal annealing experiments thanks to an original mechanism mediated by a minority charge configuration.

Influence of biaxial strain on spinodal decomposition in magnetic semiconductor alloys

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In the past few years, magnetic semiconductors (MS) - materials that combine magnetism with semiconductor behavior - have received particular interest in materials science due to their potential applications in spintronics. One well-known difficulty in the development of functional MS alloys is the limited solubility of transition metal atoms (TM) in semiconductors, which rarely exceeds a few percent, leading to second phases and TM rich regions [1]. Increasing the TM composition in these alloys is essential for developing materials with higher Curie temperatures. To overcome the formation of these embedded nanoclusters, several methods have been proposed, such as the digital delta-doping perpendicular to the growth direction [2] and the codoping of MS with shallow acceptors or donors [3].

In this work, we used spin density functional theory calculations, as implemented in the VASP code, to study the effect of biaxial strain on GaMnAs and GaCrAs [4]. The first-principles calculations have been combined with a thermodynamic analysis based on generalized quasichemical approximation (GQCA) [5]. We calculated the Helmholtz free energy, which allowed us to build the phase diagrams and obtain the critical temperatures and the miscibility gap. We show that external biaxial strain can diminish spinodal phase separation in thin GaMnAs and GaCrAs epitaxial layers pseudomorphically grown on thick unstrained zincblende (001) substrates. We studied the influence of the biaxial strain considering several fictitious substrates.

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Main Topic: T1 Density-Functional Theory beyond LDA

Atomic and electronic structure of Co2CrAl/NaNbO3/Co2CrAl magnetic tunnel junctions

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Density functional theory by means of projector-augmented-wave pseudopotential and generalized gradient approximation (PAW-GGA) method was employed to carry-out calculations of $Co_2CrAl/NaNbO_3$ interfaces. The most stable interface was found to be Co/NbO bonding geometry through comparing the formation energies of various interfaces. The half metallicity of Co_2CrAl is preserved at the interface where no interface states appear in both sides of the junction. The calculated electronic structure of Co/NbO interface shows an exchange coupling between the interface Co and Nb atoms mediated by oxygen. This interaction induces a magnetic moment of 0.053 μ_B on the interface Nb atom, which is aligned antiparallel to the magnetic moment of the Co layer. The magnetic moment of Co atom is 0.392 μ_B which is nearly a half of the bulk Co (0.730 μ_B).

Main Topic: T2 Time Dependent DFT

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

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Flavonoids and anthocyanins in particular are very attracting compounds for their roles as natural dyes (from yellow to dark blue) in plants and flowers [1], as food pigments, as antioxidant agents in drug preparations and recently as photoactive elements in dye-sensitized solar cells [2]

Here, we present a first-principles study of the effects of both hydration and thermal dynamics on the optical properties of a specific anthocyanin dye, namely, *cyanin* (Cya), in aqueous solution. We combine Car-Parrinello molecular dynamics and time-dependent density functional theory (TDDFT) [4] approaches to simulate the time evolution of UV-vis spectrum of the hydrated Cya molecule at room temperature. By the comparison of different configurations along the dynamics with and without solvent, we are able to discriminate the different effects due to the hydration and the dynamics, respectively.

The spectrum of the dye calculated in the gas phase [5,6] is characterized by two peaks in the red and in the blue, which would bring about a greenish hue incompatible with the dark purple coloration observed in nature. Describing the effect of the water solvent through a polarizable continuum model does not modify qualitatively the resulting picture. An explicit simulation of both solvent and thermal effects using ab-initio molecular dynamics [6] results instead in a spectrum that is compatible with the observed coloration. This result is analyzed in terms of the spectroscopic effects of molecular distortions, induced by thermal fluctuations.

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Main Topic: T11 Other methods

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

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In this work we present a method, based on the linearization of the band dispersion, to compute the intraband contributions to the optical spectra of metals. To investigate the performance of this method we test it on cubic iron and hexagonal magnesium. We compute the dielectric function and optical conductivity of these metals based on ab initio DFTLDA band structure, in the RPA with a full inclusion of local field effects. In particular we show that our method is capable to describe the anisotropic response of noncubic metals, without the need to resort to phenomenological parameterizations of the plasmonpole type. We also introduce a method to recover the correct asymptotic trend in the $\omega \to 0$ limit, and hence to address the static conductivity.

Dynamical response function in Sodium and Aluminum from Time-Dependent Density-Functional Theory

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We present a detailed study of the dynamic response in bulk sodium and aluminum within linear-response time-dependent density-functional theory. The results of the random-phase approximation (RPA) and the time-dependent local-density approximation (TDLDA) are poor in sodium. The approximate inclusion of the finite lifetimes of electrons and holes via a modified independent-particle polarizability greatly improves the spectra and results in very good agreement with experiment. For aluminum, the changes are less visible, but at some values of momentum transfer they are necessary to obtain qualitatively correct spectra. The double peak structure in Al is due to band structure effects but partially washed out by the lifetime effects. The latter do not, however, create a double peak by themselves as in the case of the homogeneous electron gas. Studying the performance of different time-dependent and non-local kernels we conclude that the Gross-Kohn kernel as well as the Corradini and the Hubbard local-field factors improve the spectra compared to the RPA results. However, they do not obtain an agreement close to that achieved with TDLDA and added lifetime effects. These results apply to both the spectra and the plasmon dispersion.

Main Topic: T9 Response to External Fields

First principles EPR spectra of transition metal complexes

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One of the most crucial processes for life on earth is photosynthesis, which converts solar energy into chemical energy. Light initiates a series of electron-transfer reactions that result in the water-splitting reaction, carried out in the oxygen-evolving center (OEC) of the Photosystem II (PS-II). It is generally believed that the active site of the OEC contains a Mn_4O_4Ca cluster which can exist in five oxidation states (S-states).

Although the OEC has been extensively studied by X-Ray diffraction techniques, many aspects of the molecular structure and of the oxidation reaction mechanism are still not clear, due to the limited resolution. Likewise, the interpretation of the EPR spectra of paramagnetic S-states, is hindered by the complex nature of the electronic states in transition metal complexes.

We are focusing on the development of novel theoretical methods particularly suited to study transition metal complexes, and on its application to the structure, electronic structure, and reactivity of the OEC in PS-II. Whereas plain density functional theory (DFT) fails to accurately describe transition-metal centers due to the spurious self-interaction, the DFT + Hubbard U approach has had great success in predicting difficult systems, such as the ground and excited spin states of the iron dimer.

In this work, we have studied the effect of the Hubbard U correction on the EPR spectra of simple MnO_n (n=1..4) molecules. We found that the DFT+U method improves the agreement with respect to experiment, of the EPR g-tensor and hyperfine couplings parameters. We also discuss the relation between the EPR parameters and the fine details of the electronic structure.

Finally, our results indicate the importance of benchmarking improved DFT functional (such as hybrid functionals) against the EPR spectra of transition metals complexes.

Main Topic: A3 Magnetism and Spintronics

The projector augmented–wave method: application to relativistic spin–density functional theory

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Applying the projector augmented–wave (PAW) method to relativistic spin-density functional theory (RSDFT) we derive PAW Dirac–type equations for four–component spinor pseudo wavefunctions. The PAW freedom to add a vanishing operator inside the PAW spheres allows us to transform these PAW Dirac–type equations into PAW Pauli–type equations for two–component spinor pseudo wavefunctions. With these wavefunctions, we get the frozen–core energy as well as the charge and magnetization densities of RSDFT, with errors comparable to the largest between $1/c^2$ and the transferability error of the PAW data sets. The possibilities of the theory are illustrated with some applications.

Analysis of thermodynamic, thermoelectric and magnetic properties of $FeSb_2$ in the framework of density functional theory.

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We analyze the thermodynamic, magnetic and transport properties of narrow band gap semiconductor $FeSb_2$ using the first-principles calculations based on density functional theory within the generalized gradient approximation. The vibrational properties (phonon spectrum, density of states, heat capacity) are computed through the method based on response functions calculation. The obtained results are in good agreements with inelastic nuclear scattering measurements. We therefore investigate the electron phonon coupling effects. We provide the estimations of linewidth broadening due to electron phonon coupling, along the high symmetry directions in the first Brillouin zone. The linewidth broadening seems to be much larger in the vicinity of $X(1,0,0)$ and $M(1,1,0)$ points. The values when compared to those obtained at the other symmetry points differ up to two orders of magnitude. From the Boltzmann theory applied to our GGA electronic band structure we also investigate the electrical transport properties (resistivity ρ, Seebeck coefficient S). We find that an electronic structure description is incompatible with the colossal negative value $S \approx -45000\mu V$ experimentally observed at $T \approx 10K$ [1]. We discuss here the possibility of phonons drag effects playing a significant role. The diamagnetic to paramagnetic crossover at temperature around $100K$ is also described from the calculation of the Pauli magnetic susceptibility and results are compared with experiment.

PACS numbers:

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Ab-initio investigation of lattice dynamics in substitutional disordered alloys

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To resolve the longstanding problem of calculating the phonon spectra in substituioal disordered alloys where strong force-constant disorder plays a significant role, we have devised two new first-principles based formalisms. The first one is a combination of first-principles electronic structure tools, the transferable force-constant model (TFC) of Van de Walle and co-workers (A. Van De Walle et. al., Rev. Mod. Phys. 74, 11 (2002)) and the Itinerant Coherent Potential Approximation (ICPA) by Ghosh and co-workers (S. Ghosh et al., Physical Review B 66, 214206 (2002)) while the second formalism is based on the combination of Special Quasi-random Structures (SQS) by Zunger et al. (Phys. Rev. Lett. 65, 353 (1990)) and the ICPA. We here present the salient features of these formalisms with $\mathrm{Ni}_x\mathrm{Pt}_1 - x$ chosen as an example system. Results on complete phonon spectra and related properties are presented for this alloy specimen which has significant force-constant disorder due to the large size-mismatch between the constituents.

Main Topic: A3 Magnetism and Spintronics

Magnetism & magnetic anisotropies of small structures containing 5d atoms

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The ability to enhance and tailor the magnetism of small atomic cluster and moleculeswill determine whether nanospintronics can be used as a storage technology. We present here our ab initio studies on the magnetism of small organic molecules containing transition metal atoms. We focus specially on 5d atoms like gold, platinum and iridium. These have a large spin-orbit interaction, which generates large magnetic anisotropies in small atomic clusters[1]

We present a theoretical study of the magnetic properties of the spin-1/2 dicyclopentadienyl metallocene ($M\mathrm{Cp}_2$) and phthalocyanine molecules that contain the transition-metal atoms M=Co, Cu, and Au. We find that the spin-density pattern of gold molecules shows a fully delocalized and oscillating behavior. This spin pattern is to be contrasted with the well-known cases of cobalt or iron molecules, where the magnetic moment is strongly localized at the transition-metal ion. [2]

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Main Topic: T1 Density-Functional Theory beyond LDA

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

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We have recently introduced a Koopmans correction to local and semilocal exchange-correlation functionals, aimed at linearizing the total energy wrt fractional number of electrons and able to identify orbital energies with opposite removal energies. This approach directly improves on some of the key failures of common exchange-correlation functionals, often related to self-interaction (e.g. overdelocalization of electronic states or wrong polarizability of linear chains), and provides a link between Hartree-Fock, many-body, and density-functional theory approaches to the electronic-structure problem.

We evaluate here the performance of this Koopmans correction on the electronic response, focusing on linear- and hyper-polarizabilities of linear molecules and chains. Our results indicate that the method is effective in correcting for the description of local and semi-local functionals as well as in providing eigenvalues which are in much better agreement with photoemission energies.

Main Topic: A3 Magnetism and Spintronics

First-principles study of the magnetic phase diagram of $\mathbf{LaO}_{x-1}\mathbf{F}_x\mathbf{FeAs}$

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The discovery of superconductivity in $LaO_{1-x}F_xFeAs$ with a critical transition temperature of 26 K generated considerable interest in the iron pnictides[1]. While the undoped parent compound LaOFeAs is an antiferromagnetic metal, upon doping with F the magnetic order is suppressed at $x = 0.04$, and a superconducting state arises at $x = 0.05$[2]. In this work we use density-functional theory calculations in order to investigate how the magnetic ground state evolves as a function of F content in $LaO_{1-x}F_xFeAs$. Simple models of the doping such as the rigid band approximation fail to accurately describe the relationship between fluorine content and magnetic order. We here show that by using a large supercell where fluorine atoms are explicitly included it is possible to reproduce a magnetic-nonmagnetic transition in qualitative agreement with experimental observations. We also examine the effect of the fluorine doping on the lattice parameters and we find that the dopants distort the lattice in such a way to bring the Fe and As planes closer together. We discuss the implications of our findings on the superconducting properties of $LaO_{1-x}F_xFeAs$.

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Main Topic: T2 Time Dependent DFT

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

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The investigation of the electronic structure and optical properties of DNA and DNA derivatives is of paramount importance in several scientific fields, from nanotechnology to molecular biology and drug design. In particular, circular dichroism spectra are routinely measured to characterize new structures and determine the fingerprints of specific structural motifs. Theoretical work in support of such experiments is desidered.

In this work we studied the optical signals of Watson-Crick and Hoogsteen H-bonds that are involved in the triplex formation between protonated Cytosine, Guanine and neutral cytosine. Because optical properties and transfer integrals have a strong dependence on the structure that is selected for the calculations, to bypass this limitation, we performed a Molecular Dynamics simulation to extract significant structure. We applied a clustering to generate meaningful structures from the dynamical trajectories at 300 K, thus taking into account in a simple fashion the conformational variability in the optical spectra. CDspectra have been computed for the selected structures using the `octopus` package in the framework of TDDFT in the real-time real-space implementation. We compare our results to synchroton radiation CD data measured by our collaborator Steen Nielsen and his coworkers.

Theory and Methods:

T2 Time Dependent DFT

Applications:

A1 Nanoscience

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

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An accurate description of the electronic properties of DNA is of paramount importance for all life science fields, for instance, for the study of DNA damage and repair mechanisms. One of the most common forms of oxidative damage is the replacement of guanine with 8-Oxo-7,8-dihydroguanosine (8-oxoG). In this work we investigate the electronic properties of large oligomers of single strand DNA containing either 8-oxoG or guanine bases inserted in sequences of thymines. We take advantage of recent algorithmic developments that nowadays allow to apply many body perturbation theory to very large systems up to hundreds of inequivalent atoms. The crucial idea of these developments is to exploit Lanczos techniques to avoid the calculation and the use of unoccupied states of the one electron Hamiltonian. This allows to perform GW calculations, as implemented in the QuantumEspresso package, to systems of unprecedented size. Our calculations indicate that 8-oxoG is more easily oxidized than guanine as also experimentally suggested.

Main Topic: A1 nanoscience

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

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Metal nanoparticles supported on carbon nanostructures have emerged as a new class of catalysers with interesting and potentially important applications. We present the results of first-principles Car-Parrinello molecular dynamics simulations of various model systems containing graphene, NO_2 molecules and/or Rh atoms. The goal of our study is to understand the gas-nanoparticle interactiosn and the role of the carbon surface in the chemical processes leading to catalysis. We have examined the behavior of the single rhodium atom and of clusters of 3, 10 and 20 atoms, in order to estimate the most favourable arrangements of Rh on the graphene surface. Finally, we have studied the interactions of NO_2 with the graphene-stabilized Rh clusters.

Role of the Pressure in the Elastic Properties of Ce

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Cerium "4f" electrons are peculiar in being spatially localized with a radial extent much smaller than that of 5s and 5p semicore states, yet having energy in the region of the valence 6s and 5f electrons. Two phases - alpha (α) and gamma (γ) - of cerium are under debate in terms of different properties like elastic properties or phase transition properties. The mechanical and elastic properties of cerium have generated substantial interest over the years both experimentally and theoretically. Theoretical studies, concerned with the lattice dynamics, which may be of use, as it is expected that the electron-phonon interaction plays a role during α-γ transition, are very limited. The aim of the present work is to perform a lattice dynamic and elastic constants calculations using first-principles method within linear response approach for face-centered cubic (fcc) alpha (α)- and gamma (γ)-cerium and shed some light on the interrelationship among the elasticity and phonons and understand the role of phonons in the phase transition.

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Main Topic: A7 Spectroscopies

Local Field Effects in Silicon Nanocrystals

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The effect of the local fields on the absorpion spectra of silicon nanocrystals (NCs), free-standing or embedded in SiO_2, is investigated in the framework of DFT-RPA for different size and amorphization of the samples. We show that local field effects have a great influence on the optical absorption of the NCs. Their effect can be described by two separate contributions, both arising from polarization effects at the NC interface. First, local fields produce a reduction of the absorption that is stronger in the low energy limit. This contribution is a direct consequence of the screening induced by polarization effects on the incoming field. Secondly, local fields introduce a blue-shift on the main absorption peak that has been explained in terms of perturbation of the absorption resonance conditions. Both contributions do not depend neither on the NC diameter nor on its amorphization degree, while showing a high sensitivity to the environment enclosing the NCs.

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

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As a prototype of strongly-correlated materials, NiO has been extensively studied, both by experiment and theory [1, 2, 3, 4], however, the origin of its gap is still under debate. Many-Body Perturbation Theory (MBPT) — where the key quantity is the one-particle Green's function, *aka* the propagator of an electron/hole — is the appropriate tool to study *ab-initio* photoemission gap and spectrum. The GW approximation [5] from MBPT includes dynamical correlation effects beyond H-F. The standard GW approach is not reliable on NiO since the Kohn-Sham band structure is too poor to be used as a starting point. COHSEX [5, 6] — a static approximation of GW — allows one to achieve full self-consistency, so as to obtain a better starting point for the GW step. The COHSEX+GW photoemission spectrum gives about 5 eV energy-gap, in good agreement with experiment and consistent with another more time-consuming approach beyond perturbative GW [4]. An improvement to GW would consider the screening between quantum interacting particles, adding the so-called *vertex corrections*. An attempt with the $GW\Gamma$ approximation [7] has shown no improvement in the spectrum. Possible refinements in this direction include non-locality and asymptotic constraints for the vertex Γ. Here we focus on the effects of vertex corrections on quasiparticle energies and satellites and compare the cases of Si and NiO. The Cumulant Expansion approach is discussed as an alternative method.

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Main Topic: A1 Nanoscience

Elasticity and Conductance interplay in model molecules

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Recently the interest of mechanical properties of molecules is increasing especially for it's possible biomolecular sequencing applications. Direct measurement of molecular mechanical properties (e.g. using dynamic AFM) is, however, problematic. Hence indirect methods using tunneling current obtained by STM are studied. In this work selected molecules (thio- and amino- functionalised biphenyl and octane) on gold surface are studied using DFT and Greens Function approach in order to discuss experiments and empirical model connecting molecular conductance and force response.

The effect on mechanical response (stiffness and jump to contact events) is decomposed to contributions of system parts (electrodes, linker and molecular backbone). Using this analysis explanation of several surprising experimentally observed phenomena is provided.

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

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An intriguing consequence for density functional theory (DFT) arises when considering ensembles with densities integrating to fractional particle number. The total ground-state energy as a function of particle number consists of straight-line segments and, consequently, the corresponding exchange-correlation (XC) potential jumps discontinuously. This feature of the exact theory turns out to be a key property to incorporate in approximate functionals in order to obtain, e.g, accurate band-gaps of solids and correct molecular dissociation limits.

It has been demonstrated that the discontinuous nature of the static XC potential naturally carries over to the XC potential of time-dependent density functional theory (TDDFT) appearing in, e.g., time-resolved ionization processes. How the same property is reflected in the XC kernel, defined as the functional derivative of the XC potential with respect to the density, has, so far, not received any attention. The XC kernel is of fundamental importance in TDDFT as it gives access to the particle conserving excitation spectrum. In this work we have investigated the discontinuities of the XC kernel and found them to be crucial for the description of long-range charge-transfer excitations.

Formalism for GW calculations without empty states in a localized basis

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We present a formalism to perform GW quasi-particle calculations without performing expansions over unoccupied states and using a local orbital basis. This formalism is expected to open the way to GW calculations showing a more favourable scaling with system size as compared to the traditional N^4 scaling. In order to avoid the expansion of the screened Coulomb interaction and the non-interacting Green's function over empty states we solve self-consistently a linear-response Sternheimer equation.[1] While the original proposal was based on a plane waves basis representation, we here explore the possibility of further improving the scaling properties of this scheme by using localized pseudo atomic-orbitals as a basis.[2] In our proposed scheme the screened Coulomb interaction, the non-interacting Green's function, and the GW self-energy are represented in such local basis and inherit the sparsity of the Kohn-Sham one-particle Hamiltonian. We here examine the advantages and pitfalls of excited state calculations within a local orbital representation and we discuss solutions to achieve accuracy comparable to plane-wave GW calculations.

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Ab initio investigation of topological insulators

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Since the successful mechanical exfoliation of graphene in 2004, a new field of materials science and condensed matter physics emerged. Graphene is a strictly 2D material that exhibits unique electronic, thermal, and optical properties making it a "wonder material" with potential applications. Its electrons behave like massless Dirac fermions with linear electronic dispersion at the Dirac point. This new exciting physics caused a "graphene hype" in the material scientists community and most of the experimental and theoretical efforts have focussed on graphene.

Very recently, atomically-thin crystalline films and ribbons of bismuth telluride have been obtained by exfoliation of crystalline Bi_2Te_3 [1]. Bulk Bi_2Te_3 is a material with extraordinary thermoelectric properties and its doping with Sb or Se resulted in very high thermoelectric figure of merit (ZT) values. It has also been indicated that the ZT value can be enhanced by the low-dimensional structuring of BiSbTe alloys. Moreover, stacked 2D layers of Bi_2Te_3 as well as Bi_2Se_3 and Sb_2Te_3 were recently identified as promising topological insulators [2]. This experimental findings highly motivated the present ab initio investigation of 2D crystals. In particular the electronic properties of bulk Bi_2Te_3, Bi_2Se_3, and Sb_2Te_3 as well as their 2D analogues are calculated within density functional theory using hybrid functionals and taking into account relativistic effects of the valence electrons. In a slab geometry, the dependence of the electronic gap on the slab thickness is studied and compared to experimental findings.

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Linear Response TDDFT in CASTEP: An HPC Implementation

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We present an efficient and parallel implementation of linear response time-dependent density functional theory (TDDFT) in the plane wave pseudopotential code, CASTEP. Our work is based on Hutter's [J. Chem. Phys. **118**, 3928, (2003)] implementation within the Tamm-Dancoff approximation. Many adiabatic exchange-correlation functionals are available, including popular hybrids PBE0 and B3LYP and also, by extension, CIS. A customised block-Davidson algorithm was used, which is particularly suitable for the solution of large eigenvalue problems in high performance computing (HPC) environments. Using two parallel distribution schemes, efficient scaling can be achieved beyond 1000 processing elements. Excitation energies and partial optical spectra of small to medium-sized molecules are shown.

Main Topic: T9 Response to External Fields

Total Energy Formalism for Charged Nanocapacitors: Orbital Partition Approach

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The understanding and control of the capacitance of nanostructures is one of the key issues for further scaling of nanodevices. The calculation of capacitance requires the charging of a metal/insulator/metal (MIM) structure under applied bias voltage, but this is incompatible with the conventional Kohn-Sham (KS) formalism of density functional theory (DFT) which seeks the global ground state. Several methods have been proposed to extend KS-DFT for the consideration of applied bias, but these methods have not seen widespread use due to limitations in accuracy and/or efficiency, geometric constraints, and difficulty in implementation.

In order to rectify this situation, we propose a novel but simple alternative that is based on the partitioning of the KS orbitals around the Fermi level into metal and insulator parts. The partitioned orbitals are occupied according to different Fermi levels, allowing for the consideration of bias voltage in a straightforward manner. The self-consistent loop procedure is carried out in the same manner as in conventional KS-DFT calculations. Thus, we can define and calculate unambiguously the total energy of a nanocapacitor that is charged through the application of a specified bias voltage.

We implemented this method within VASP code [1], and performed calculations on Au(100)/MgO(100)/Au(100) nanocapacitors of various dielectric thicknesses (ranging from about 1.5 nm to 4 nm). The capacitance was evaluated by $C = 1/V\, dE/dV$ at $V = 0.6$ V (dE/dV was calculated from total energies at 0.5, 0.6, and 0.7 V using finite differences). The inverse capacitance of this system is found to be linear with respect to thickness d ($1/C = d/A(\varepsilon_0\varepsilon_b)$ + const.). The bulk dielectric constant evaluated from the slope is 9.33, which is identical within numerical accuracy to the value 9.59 calculated from density functional perturbation theory in a bulk model. Thus we can be fairly sure that the energy and forces are calculated accurately using this method. Furthermore, the intercept was slightly negative, indicating that the capacitance is slightly larger than that calculated from the bulk dielectric constant. This is in agreement with a previous work which calculated the capacitance from the polarization induced by a constant external field [2].

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Electron-electron interactions in superconducting Lithium under pressure

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Lithium is known to exist in different phases under pressure and known to superconduct under pressure. We look at the screened electron-electron interactions in Lithium by diagnolizing the dielectric matrix $\epsilon^{-1}_{GG'}$(q,ω) and obtaining the dielectric band structure at different q points. We analyze the eigenmodes of $\epsilon^{-1}_{GG'}$(q,ω) for different q. We look at the differences in the eigenmodes of the dielectric matrix by subjecting lithium to pressure. We also do the analysis for different crystallographic phases of lithium under pressure. Even though the superconductivity in lithium is electron-phonon mediated, lithium is a good test system to study the screened e-e interactions as this might be a primary mechanism for superconductivity in high T_c nitrides of the form MNCl (M=Ti,Zr,Hf).

PACS numbers:

Main Topic: T8 Electronic Transport

Resolving Controversies on the Multiple Conductance Peaks in Single-Molecule Junction Experiments by Multiscale Simulations

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The key difficulty in interpreting single-molecule junction experiments arises from the uncertainties in molecule-metal contact configurations. They are hardly revealed in experiments, and in this regard theoretical approaches are required to resolve the problem. In our previous study, applying a multiscale computational approach that combines force fields, density functional theory, and matrix Green's function calculations [1], we observed a single conductance peak for a haxanedithiol (C6DT) molecule thermally fluctuating between flat Au(111) electrodes [2]. In this report, we extend our previous work and consider the thermally fluctuating C6DT molecule on a series of Au surfaces with different number of adatoms. By studying more realistic molecular-metal contact geometries, we find that the mobility and coordination number of S-Au complexes is the key in explaining the current experimental controversies on the multiple conductance peaks.

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Main Topic: T1 Density-Functional Theory beyond LDA

Expanded radialenes carbon nanotubes: electronic and elastic properties

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Abstract. The series of expanded radialenes of molecular formulae $C_{2n}H_n$ and $C_{3n}H_n$ are obtained by inserting acetylene or diacetylene groups between each pair of methylene units of radialenes C_nH_n. This paper reports on the new theoretical investigation of electronic and elastic properties of some carbon nanotubes based on expanded radialenes with different diameters and with the armchair and zigzag edges. Using the ABINIT software package, which is based on the Density Functional Theory (DFT), we found that all studied carbon nanotubes based on expanded radialenes possess metallic behavior. Also, the calculations show that the elastic properties of the nanotubes strongly depend on the form of the rolling up (armchair *(m,m)* or zigzag *(m,0)*). The Young's modulus is slightly smaller for the *(m,0)* nanotubes and a bit larger for *(m,m)* nanotubes. The zigzag carbon nanotubes based on expanded radialenes are energetically more stable than C_{60} while armchair ones are less stable than C_{60}.

Note: Please choose one of the following as "Main Topic" above:

Theory and Methods:
T1 Density-Functional Theory beyond LDA

Applications:
A1 Nanoscience

Main Topic: A7 Spectroscopies

Determination of NMR chemical shifts for cholesterol crystals from first-principles

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Solid State Nuclear Magnetic Resonance (NMR) is emerging as a powerful tool in crystallography. The wealth of important information available from spectroscopy, however, cannot be extracted from the experimental data alone. Experimental spectra present a set of peaks which need to be compared with theoretical predictions for an unambiguous identification. So far, several empirical methods have been employed for the interpretation of the measured spectra. However, many interesting systems are outside the scope of these empirical methods due to their complexity. Therefore, *ab initio* approaches, such as the gauge including projector augmented plane wave (GIPAW) approach, stand out as a valuable tool for determining NMR spectra, even for complex systems. The applicability of GIPAW in large systems is limited only by the feasibility of the calculations. Our recent implementation of ultrasoft and projector augmented wave (PAW) pseudopotentials within GIPAW method in Quantum Espresso simulation package allows affordable *ab initio* calculations of NMR chemical shifts for systems of the order of thousands of electrons.

After presenting an evaluation of the method, we report the first *ab initio* determination of NMR spectra for several crystal structures of cholesterol ($C_{27}H_{46}O$) molecules. Cholesterol crystals, the main component of human gallstones, are of interest to medical research as their structural properties can shed light on the pathologies of gallbladder. With our application we show that *ab initio* calculations can be employed to aid NMR crystallography in this important research field.

Main Topic: T1 Density-Functional Theory beyond LDA

Pressure induced unified study of strongly correlated ErSb

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Abstract

The magnetic, electronic, structural and mechanical properties of ErSb in the stable Fm$\bar{3}$m and high-pressure Pm$\bar{3}$m phases have been analyzed by using the full potential linear augmented plane wave method (FP-LAPW) employing the LSDA +U scheme (local spin-density approximation with Hubbard-U corrections) within the framework of density functional theory. The spin–orbit coupling (SOC) has been taken into consideration. The magnetic phase stability has been determined from the total energy calculations for both the non-magnetic and magnetic phases which show that ErSb is ferromagnetically stable at ambient and high pressures. Under compression ErSb undergoes first-order structural transition from B1 to B2 phase at 24.56 GPa which shows good agreement with the experimental value of 25 GPa, respectively. The elastic properties of ErSb have also been computed at normal and high pressures. The structural properties *viz*, equilibrium lattice constant, bulk modulus and its pressure derivative, transition pressure, volume collapse and elastic moduli agree well with the experimental data. The electronic structure at different volumes is investigated with on-site Coulomb potential (U) for the Er-derived 4*f* orbitals to obtain the correct ground state of ErSb. These calculations showed that all the three compounds are half metallic in their ground state. The LSDA+U strategy shows significant impact on the energy levels of the occupied and unoccupied 4*f* states of ErSb. A detailed analysis shows that the LSDA+U method provides the better description of our systems.

Direct calculation of the one particle Green's function: an alternative to the self-energy

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Calculations of quasi-particle band structures and photo-emission spectra of materials rely more and more on perturbative many-body techniques like the GW approximation. In this approach the one-body Green's function (G) is determined from a Dyson equation containing a *self-energy* kernel Σ which is approximated as a product of G and the screened Coulomb interaction W. To go beyond the first order in W, iterative schemes of Hedin's equations [1] have been proposed. While generally successful, GW is known to fail for strongly correlated systems, and it is far from obvious that one could improve on this through further iterations of Hedins equations and vertex corrections to Σ. In the present work we explore an alternative route: in place of approximatingΣ , we reformulate the problem in terms of a set of coupled rst order differential equations (ODEs) for the unknown G. We first employ a 1-point workframe, in which we solve exactly the -now algebraic- ODE for G. This allows us to **i)** understand some of the main issues of the approach, particularly how to solve the ODE's initial valuse problem; **ii)** benchmark, within the 1-point frame, different many-body perturbative schemes such as the iteration for the differential equation itself, G_0W_0 , G_0W_0 towards self-consistency and vertex correction such as $GW_0\Gamma$, $GW_0\Gamma_0$; **iii)** obtain insights concerning the N-points solution.

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Electronic correlations at the α-γ structural phase transition in paramagnetic iron

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We present an application of a novel *ab initio* approach to calculate the total energy of materials with correlated electrons [1]. It combines band structure and dynamical mean-field theory, and is implemented in terms of plane-wave pseudopotentials. Here we employ this computational scheme to study structural and magnetic properties of elemental Fe at finite temperatures [2]. For this purpose we analyzed the energetics of the *bcc*-*fcc* lattice transformation in Fe using the Bain transformation path. We find that at ambient pressure the temperature of the *bcc*-*fcc* structural phase transition occurs at ∼200 K above the calculated Curie temperature. The structural optimization performed for paramagnetic Fe yields the correct lattice constants and predicts a 2 % shrinking of the volume at the *bcc*-*fcc* phase transition. The phonon dispersion of paramagnetic *fcc* iron shows good agreement with experimental data.

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Main Topic: T9 Response to External Fields

High-pressure Raman spectra of TiO_2

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Intensities of Raman lines are important part of the information contained in the vibrational spectra of crystals. Due to the changes in the crystal structure as a response to external perturbation (like pressure or temperature), the frequencies, as well as the intensities of Raman active modes change under external influence. The intensity of Raman lines are important information about the properties of studied system, but are usually not used very much.

A Raman study of a oriented single crystal gives information about the components of Raman tensor for various Raman active modes. We calculated intensities of Raman modes of tetragonal rutile structure with space group $P4_2/mnm$ of TiO_2 crystal at various pressures. The ABINIT density functional program package is used for the calculation of vibrational frequencies and Raman tensor components. The values given by calculations are in a fair agreement with the observed positions of phonons as a function of pressure. The possibility to use Raman intensities as additional tool in the study of phase transitions is discussed.

Main Topic: A3 Magnetism and Spintronics

Magnetism in FeMn Nanostructures

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The magnetic structure of ultrathin films FeMn ordered alloy on Cu(001) substrate is investigated by a first principle self-consistent pseudopotential plane waves method. It incorporates intra-atomic noncollinear magnetism in order to understand the magnetic complexity involved in the spin-flop coupling. The occurrence of a noncollinear magnetic structure is predicted. For 1-ML Mn/1-ML Fe on Cu(001), we found that the ground state corresponds to a ferromagnetic order between Fe moments and the Mn moments on the neighboring sites making an angle of 185°. For Fe[110]/Mn[110] ordered rows, an antiferrimagnetic coupling between Mn atoms and canted Fe moments making an angle of 11.6° have been obtained. Whereas, a ferromagnetic (an antiferromagnetic) coupling between Fe (Mn) atoms is predicted for Fe[010]/Mn[010] ordered rows. A tentative explanation of these results is proposed.

Main Topic: T1 Density-Functional Theory beyond LDA

Study of the relaxation of the Aluminum cluster in the self-compressed inhomogeneous stabilized jellium model

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The bond lengths of atoms in a cluster composed of a few atoms may vary, in general, with the number of atoms. If the number of atoms is sufficiently high that some of them constitute the bulk region, then the average bond length in the bulk may differ from that in the surface region.

Treating the ions in the jellium model, the average bond length of atoms would have an intimate relation with the jellium density, and thereby, the jellium densities in the two regions may differ. To describe the inhomogeneity in the jellium density, we have used the self-compressed inhomogeneous stabilized jellium model.

In this work, we have applied the self-compressed inhomogeneous stabilized jellium model to a 30-atom aluminum cluster. Using the bulk density parameter of $r_s^{bulk} = 2.07\ (au)$ for Al, we have calculated the inner region density parameter equal to $r_s^{in} = 2.57\ (au)$ and for the surface region equal to $r_s^{out} = 1.97\ (au)$. This means that the jellium density in the inner region has been decreased while that in the surface region has been increased relative to that of infinite bulk. This result is consistent with those obtained for aluminum thin films.

RVB states in graphene and other carbon compounds

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We study the relevance of the resonating valence bond (RVB) wave function for describing the ground state and the low energy properties of carbon compounds. We consider three different systems of increasing interest: the simplest carbon dimer, the benzene, i.e. the prototype molecule of the resonance valence bond, and the ideal two dimensional graphene layer. The RVB wave function considered here is the product of a Jastrow factor and an antisymmetrized geminal power (JAGP), with an appropriate constraint on the number of partially occupied molecular orbitals. For C2 and benzene we consider the binding energy and compare the RVB results with the ones obtained with a standard Jastrow correlated Hartree Fock wave function. We show that the "resonance energy" captured by the JAGP allows to achieve a much better agreement with the experimental data in the C2 case. For benzene, the binding energy is overestimated, however we are able to recognise the resonating Kekulé and Dewar structures. Finally, for graphene we perform the first ab initio QMC investigation of the possible stability of an RVB state characterized by an s-wave or d-wave pairing function.

Main Topic: T4 Quantum Monte Carlo

Spin and valley susceptibility in wide AlAs quantum wells.

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We have performed extensive diffusion Monte Carlo simulations for a two-dimensional electron gas with a mass anisotropy appropriate to AlAs quantum wells. We consider both the strictly two-dimensional limit and thicknesses encountered in actual devices, as well as one and two-valley systems. We demonstrate that in the one-valley case anisotropy suppresses the enhancement of the spin susceptibility substantially at all densities and in particular at those relevant to experiments, the effect being larger at lower density. This suppression adds onto the one due to thickness. In the two-valley case we find an interesting interplay of the anisotropy and the valley degree of freedom in determining the electron gas properties and in particular the spin susceptibility. We find a good agreement between our predictions and the available experimental evidence, pointing to a minor residual role of disorder on the spin susceptibility enhancement at low density in the one-valley devices. Finally, we discuss the role of the mass anisotropy, the thickness, and the spin and the valley polarisation in the determination of the valley susceptibility.

A self-consistent, first-principles method for complex disordered materials

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The coherent potential approximation[1] (CPA) provides a powerful method for ab initio investigations of materials with disorder, such as metallic alloys, doped semiconductors, and magnetic systems in paramagnetic phases above their Curie temperatures. Fully self-consistent results can be pursued over the whole range of constituents' concentrations, without the typical limitations of supercell approaches. Proper accounting of short range ordering effects (SRO) and other local environment features can also be achieved through the theory's recently proven non-local extension[2] (NLCPA), in which simple systems with one atom per unit cell lattice structures are described by means of a self-consistent effective medium with correlations over appropriate length scales built in. For complex multi atom per unit cell materials, selective disorder scenarios can be studied through the independently developed multisublattice reformulation[3] of the CPA (MSCPA), which retains however the original limitations of a single site treatment.

Here we propose a generalisation of the NLCPA idea to crystalline materials with multiple atoms per unit cell lattices. The method is illustrated using a simple tight-binding model, and then given in a Korringa-Kohn-Rostoker (KKR) multiple scattering implementation for a general ab initio density functional investigation of disorder. Results are first discussed with reference to the topical example of changes in the electronic structure of a CuZn alloy as the SRO of its homogeneously disordered phase transforms towards clusters segregation or long range ordering. This paves the way to treating more complicated systems of immediate technological interest, such as doped semiconductors and oxides beyond a cubic structure.

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Main Topic: A3 Magnetism and Spintronics

MICROMAGNETIC SIMULATIONS OF FIELD INDUCED DOMAIN WALL MOTION IN $Fe_{20}Ni_{80}$/Cu/Co SPIN VALVE

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ABSTRACT

Using numerical micromagnetics simulations, we have investigated domain wall motion in $Fe_{20}Ni_{80}$/Cu/Co spin valve. In that system, a layer of $Fe_{20}Ni_{80}$ containing a transverse head-to-head domain wall is coupled to a uniformly magnetized Co layer, via a non magnetic Cu layer. We computed the static equilibrium magnetization distribution and showed that the wall in $Fe_{20}Ni_{80}$ widens, compare to that of a single $Fe_{20}Ni_{80}$ nanostrip, while a quasi-wall is created in the Co layer. Thereafter, we investigated the domain wall dynamics in detail, under an applied magnetic field.

First-principles Study of P3HT/ZnO Hybrid Organic-Inorganic Photovoltaic Interface

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Hybrid organic-inorganic photovoltaics have been the focus of intense scientific interest in recent years[1,2]. By using a combination of a conducting organic polymer and an inorganic semiconductor, hybrid photovoltaics enable the possibility of large-area, low-cost solar energy conversion – something that conventional photovoltaics, despite their high efficiencies, have been unable to achieve. Hybrid photovoltaics comprised of P3HT and ZnO have attracted considerable interest due to the possibility of solution processing and the favourable interfacial energy level alignment. Despite the tremendous progress that has been made in enhancing device efficiencies, much improvement remains if P3HT/ZnO hybrid photovoltaics are to become commercially competitive. We present here a first-principles investigation of the photovoltaic interface of P3HT and ZnO. Using a density-functional approach, we study the structure and energetics of model interfaces between ZnO and P3HT[3], and we identify possible binding configurations of the polymer on the ZnO surface. This work provides a solid basis for investigating the impact of the binding mode on the interfacial charge transfer, which is critical in determining the performance of a hybrid device. In order to address the shortcomings of standard DFT in calculating band offsets, we present preliminary corrections to the electronic structures of P3HT and ZnO using hybrid functionals[4].

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Main Topic: A3 Magnetism and Spintronics

p Magnetism in CaC: First principle study

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On the basis of density functional theory (DFT) calculations, we study electronic, magnetic and structural properties of the high ionic CaC compound in 6 different phases: Zinc Blend, Rock Solt and B_2 with cubic structure and Wortzite, NiAs, and r-NiAs with hexagonal structure. A ferromagnetic equilibrium state was found in the RS, NiAs, WZ, and ZB structures of this non-transition metal compound. Analyzing of electronic structure indicates that ferromagnetism in this ionic compound originate from the flat p orbital of anion atom (Carbon) around the Fermi level, as describe by Hund's rule. Moreover, we observed that this compound shows half metalic behavior in the equilibrium ZB and expanded WZ structures indicating potential applications of these systems in spintronics devices. The topological analysis of electronic charge density is employed to study the magnetic phase transitions of CaC in the selected structures. It was found that the paramagnetic-ferromagnetic phase transition in B2 structure is accompanied by a topological transformation of electron density while the ferromagnetic-half metallic transtions in RS and ZB structures are associated with geometrical transformation of electron density.

Main Topic: A1 Nanoscience

Stability of domain boundaries on the Ge-covered 5×5-reconstructed Si(111) surface

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Extended one-dimensional defects, such as steps or domain boundaries, can be used to template nanostructures. In particular, with solid phase epitaxy, the Ge/Si(111) system can be prepared with a high density of 5×5 domains. The domains are in-registry with the substrate but translationally shifted with respect to each other, meeting at atomically ordered, linear boundaries. These boundaries can be used to template linear arrays of Ge or In "magic" clusters (clusters of uniform size and structure) [1]. We will present a theoretical study based on first-principles total-energy DFT calculations and simulations of scanning tunneling microscopy, which corroborates the previous experimental findings. We aim to explain the intriguing distribution of domain-boundary types found in the experimental study. We optimize the structures of the domain boundaries that have been proposed on the basis of the experiments. Different models of the boundaries are compared in terms of line tension (essentially an excess energy of the boundary per unit length) obtained from large-scale DFT calculations. In order to carry out the calculation, which requires up to several hundreds of atoms in a unit cell, we make use of the `FIREBALL` computer code [2]. Additionally, a simple analytical model has been established to describe the effective interaction between domain boundaries. The results of our study—and, from a larger perspective, the general methods that we have developed for this particular case—will produce a deeper understanding of nanostructure growth at domain boundaries.

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First-principles study of O1s core-level shifts at dye-sensitised solar cell interfaces

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Dye-sensitised solar cells (DSCs) employing mesoporous TiO_2 films sensitised with ruthenium-based dyes have shown consistently good performance over the last two decades. Understanding the process of charge injection in these devices requires detailed atomic-scale models of the interface between the light-absorbing dye molecule and the semiconducting substrate. Despite considerable efforts devoted to the experimental[1,2] and theoretical[3,4] investigation of such interfaces, different viewpoints still exist regarding their atomistic nature. We have performed density-functional theory calculations of the O1s core-level shifts[5] in order to interpret photoemission data reported for a ruthenium sensitiser/anatase(101) interface[2]. We show that the core-level shifts provide a useful probe into the nature of bonding at the interface and can be used to successfully interpret the measured spectral features.

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Nonlinear Elasticity of Graphene and Other Hexagonal Carbon Allotropes

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Carbon allotropes characterized by sp^2 hybridization have recently attracted much attention due to the experimental availability of single-layer graphene sheets [1]. In particular, the elastic properties of graphene have been found to be extraordinary, establishing graphene as the strongest material ever measured [2]. Additionally, graphene shows a remarkable nonlinear elastic behaviour [2,3]. In this work, we present a first-principles study of the linear and nonlinear elastic properties of diamond, graphene monolayers, as well as simple-hexagonal, hexagonal, and rhombohedral graphite. Calculations are performed using the pseudo-potential density-functional-theory code Quantum ESPRESSO (QE) [4] and both the local-density and generalized-gradient approximations for the exchange-correlation energy. For each system, the Lagrangian stress tensor is calculated for distorted structures defined by given values of the Lagrangian strain. The investigation of the stress dependence on the strain allows the determination of second and higher-order elastic constants. The results we have obtained for elastic constants at different orders are discussed in comparison with experiment [2] and previous calculations [3] and with second- order results achieved using the full-potential LAPW code WIEN2k [5]. In particular, we consider the issue of numerical accuracy in the ab-initio calculation of higher-order elastic constants. Furthermore, we investigate the role of van-der-Waals interlayer interactions by using the vdW-DF extension [6] to the QE software package.

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Main Topic: A1 Nanoscience

Ab-initio calculations of absorption spectra of nanowires by solving the Bethe-Salpeter Equation

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A first principle approach to the solution of the Bethe Salpeter equation without empty electronic states has been recently developed [1], which makes possible the calculations of absorption spectra of relatively large systems (with several hundreds of electrons). We present applications of this approach to quasi-one dimensional systems, including chains of hydrogen molecules and Si nanowires. We discuss techniques to further improve the performance of absorption spectra calculations, and present a general scheme to accurately integrate the divergence in the screened exchange integrals. Finally, in the case of Si nanowires, we discuss the effect of surface reconstruction in shaping optical absorption spectra.

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Main Topic: A11 Density-Functional Theory beyond LDA

Dispersion interactions in room-temperature ionic liquids: Results from a non-empirical density functional

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The role of dispersion or van de Waals interactions in imidazolium-based room-temperature ionic liquids is studied within the framework of density functional theory, using a recently developed non-empirical functional [1], as efficiently implemented in the SIESTA code [2]. We present results for the equilibrium structure and lattice parameters of several crystalline phases, finding a general improvement with respect to both, the local density (LDA) and the generalized gradient approximations (GGA). In particular, equilibrium volumes reproduce experimental values to unprecedented accuracy. Intra-molecular geometries are retained, while intermolecular distances and orientations are notoriously improved relative to LDA and GGA. The quality is superior to that achieved with tailor-made empirical *ad hoc* VDW corrections [3]. We provide some insight into the issue of polymorphism of [bmim][Cl] crystals, and we present results for the geometry and energetics of [bmim][Tf] and [mmim][Cl] neutral and charged clusters, which validate the use of empirical force fields. By comparing to quantum chemical MP2 calculations on clusters, we validate VDW geometries and more importantly binding energies. We also analyze the performance of an optimized version of this non-empirical functional, where the screening properties of the exchange have been tuned to reproduce high-level quantum chemical calculations [4].

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Main Topic: A1 Nanoscience; A6 Surfaces; A3 Magnetism and Spintronics

Edge effects in graphene nanoislands on Co(0001)

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We recently demonstrated the growth of regularly shaped, nanoscale graphene islands of graphene on Co(0001) surfaces [1]. Here we combine low-temperature scanning tunneling microscopy (STM) measurements and DFT based calculations to study their edge properties. These graphene nanoislands reveal a well-ordered structure at the edges, with predominant zigzag termination. STS tunneling spectra show prominent peaks at low bias, where the edges dominate the images. DFT calculations provide insights into the relative stability of different edge configurations and passivation conditions, as driven by interactions with Co. The coupling with the substrate results also in a dramatic modification of both electronic and magnetic properties at the edges. In order to study hybridization and size effets, we transform to localized Wannier states and develop a minimal model for the effective π states of these graphene nanostructures.

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Main Topic: Magnetism and Spintronics

Surface-induced magnetism in C-doped SnO_2: First-principles study

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The magnetism of C-doped SnO_2 (001) surfaces is studied using first-principles calculations. It is found that carbon does not induce magnetism in bulk SnO_2 when located at the oxygen site, but shows a large magnetic moment at the SnO_2 (001) surface. The magnetic moment is mainly contributed by the carbon atoms due to empty minority spins of p orbitals and is localized at the surface and subsurface atoms. No magnetism is observed when the carbon atom is located at the subsurface oxygen sites. The origin of magnetism is discussed in the context of surface bonding.

Monte Carlo modeling of structural properties in compressed 2D Wigner crystals

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We present a numerical modeling of the formation of ordered structures and the structural transitions within 2D few-particle systems. Strong interaction forces lead to the formation of ordered structures (Wigner crystallization). It is observed in numerous systems as quantum dots, electrons on liquid He, ions in traps, dusty plasmas, macroscopic model systems [1]. Under different conditions such systems undergo the erosion or reorganization of the structure. The macroscopic definitions of phase transitions are ambiguous for the few-particle systems [2].
In this work the structural transitions within 2D systems up to 10 particles caused by squeezing of the confinement potential are modelled using the statistical Monte Carlo technique with optimizing algorithms. The particles interact through Coulomb repulsion forces and are confined by a parabolic potential $V_c = x^2 + \alpha^2 y^2$. Departure of the parameter α from unity squeezes the potential inducing structural transitions. The dependence of the specific heat C_v of the system, estimated from statistical energy fluctuations, upon the confinement potential is explored. Sudden changes of C_v signal the structural and symmetry changes, that play the role of phase transitions in a finite system.

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Main Topic: A1 Nanoscience

Surface-induced atomic and electronic properties of unpassivated GaAs Nanowires

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Semiconductor nanowires (NWs) are particularly interesting for applications to nanoelectronics and nanophotonics, owing to their one-dimensional structure, and to the large surface to volume ration [1]. A number of key renewable energy applications, such as photoelectrochemical water splitting, and solar cells, have also been devised for nanowires, together with applications to nanosensoring for environmental pollution detection and antibody molecule recognition [2,3].

Based on accurate ab-initio calculations, we propose a model for predicting the stability of III-V Nanowires (NW) having different sidewalls and ridge configurations. The model allows us to obtain the NW formation energies performing calculations only on relatively “small” systems: small diameter NWs and flat surfaces, to extract the contributions to stability of each structural motif. The method can be applied generally also to other differently shaped and oriented III-V NWs. The model shows that NW surfaces mainly determine the NW stability, so as the changes to the surface structure would modify the final NW structure in a remarkable way. We find that wurtzite and zincblende nanowires have similar energies over a wide diameter range, thus explaining the observed polytypism. Furthermore, new more stable ridge reconstructions are proposed for zincblende nanowires. The surface related structural motifs have also clear fingerprints on the NW electronic structure: the more stable nanowires are all semiconducting; the bandgaps are ruled by surface states and do not follow the trend mandated by the quantum confinement effect; small diameter wurtzite nanowires have an indirect band gap, but for some of them an indirect to direct transition can be foreseen to occur at larger diameters. Surface states have a larger impact on the zincblende NW bandgaps than on the wurtzite NW ones.

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Main Topic: T3 Many-Body Techniques for Real Materials

Electronic properties of crystal and amorphous phases of SiO_2: disorder effects within and beyond Density Functional Theory

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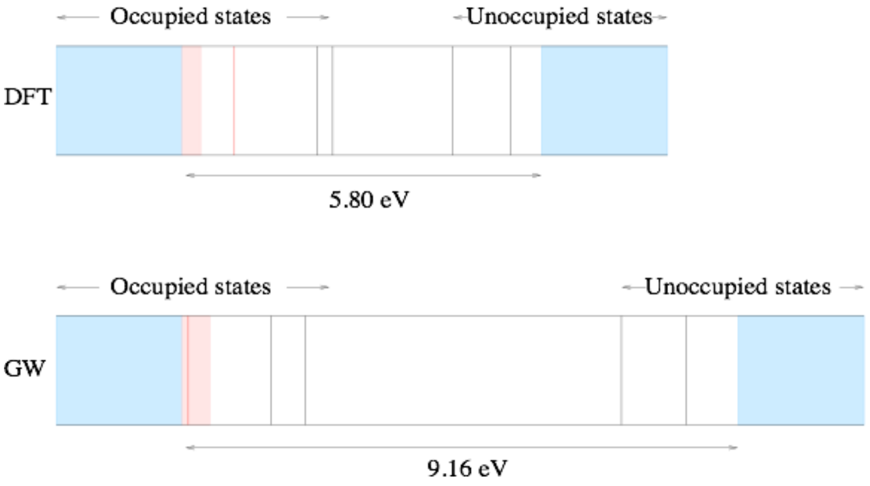
We present a first-principles systematic study of the electronic structure of SiO_2 including the crystalline polymorphs (quartz and cristobalite), and different types of disorder leading to the amorphous phase. We start from calculations within density functional theory and we then proceed to more sophisticated many-body perturbation theory calculations within the *GW* scheme. We show that the mobility gap of amorphous silica coincides with the band gap of quartz, contrary to the traditional picture and to the density-functional theory results. Our results [1] show that different kinds of disorder have also different impact on atomic and electronic-density fluctuations, which affect the electronic structure and, in particular, the size of the mobility gap. The inclusion of the local field effects in the exchange-correlation potential turns out to be crucial to quantitatively describe amorphous systems and defect states.



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Main Topic: T1 Density-Functional Theory beyond LDA

DFT and Beyond - Climbing Jacob's Ladder

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Density functional theory (DFT) has shown to be an efficient method to calculate a wide range of materials properties. Nevertheless, no DFT-functional yields satisfactory and accurate answers for all physical problems. We investigate the performance of various DFT- and beyond DFT methods for lattice constants, heats of formation and atomization energies. Specifically, we will show results for LDA, PBEsol, HSEsol (a hybrid based on PBEsol) and the random phase approximation (RPA) within the adiabatic connection fluctuation dissipation framework (ACFD), each of which represents a rung in Perdew's Jacob's Ladder[1].
Furthermore, we present ab-initio calculations of the zero-point anharmonic expansion (ZPAE) effect on the lattice constants. The increase of the theoretical lattice constants caused by ZPAE can be as large as 2%. In the view of very accurate methods like the RPA (average lattice constant error smaller than 0.5%) this effect must not be neglected. We show that it is sensible to correct the experimental lattice constants using corrrections calculated at the PBE level.

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Main topic: T1- Density functional theory beyond LDA

Polynitrogen confined to C60 Cage: A novel energetic Material

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In recent years, interest in polynitrogen or polymeric nitrogen has drawn considerable attention not only because of its theoretical significance but also because of its possible application as a high energy density material (HEDM)[1,2]. Polynitrogen molecules are formed by a combination of lower-order bonds, and while decaying into dinitrogen (N_2) molecules, they release enormous amount of energy and are environmentally safe. Over the last few decades, there have been consistent efforts to predict new exotic forms of all-nitrogen molecules using various experimental and theoretical techniques [3,4].

Therefore, in this problem using density functional theory, we have explored the possibility of trapping polynitrogen clusters inside C_{60} fullerene cages. Our results indicate that C_{60} can act as an ideal candidate to trap nitrogen in polymeric form. We found that a maximum of 13 nitrogen atoms can be encapsulated in a C_{60} cage without distorting the C_{60} cage significantly. The nitrogen clusters in confinement exhibit unique stable structures in polymeric form, mostly in single and double-bonded formations. The $N_n@C_{60}$ molecules retain their structure, even at 300 K, for $n \leq 12$. The Mulliken charge analysis shows a very small charge transfer in $N@C_{60}$, consistent with the quartet spin state of N. However, for $2 < n < 10$, charge transfer takes place from the cage surface to the N_n compounds, and inverse polarization thereafter.

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Main topic: T11- Other Methods

A unified pseudopotential approach to superconducting state parameters of Mg, B and MgB_2

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Abstract : Pseudopotential theory has been applied in BCS-Eliashberg-McMillan framework by employing T_c-equation due to Allen and Dynes for estimation of superconducting state parameters, viz., electron-phonon coupling strength (λ), Coulomb pseudopotential (μ*), transition temperature (T_c), isotope effect exponent (α) and interaction strength (N_oV) of Mg, B and MgB_2 in a unified approach for the first time. The empty core model pseudopotential due to Ashcroft and RPA form of dielectric screening function due to Linhard are used, which provide superconducting state parameters of Mg and B in excellent agreement with the relevant experimental data and other theoretical results. Form factors of MgB_2 , computed from the form factors of component metals (Model-I), are used for theoretical estimation of superconducting state parameters of MgB_2. The T_c value of MgB_2 (39.126 K) obtained from the this approach shows an excellent agreement with the other theoretically computed values of T_c and the relevant experimental data. The explicit dependence of λ and T_c on the isotopic mass of Mg and B, as revealed from the present work, confirms the role of lattice vibrations in the superconducting behaviour of MgB_2 and the high value of T_c in it may be attributed to the phonon-mediated e-e interaction coupled with higher values of phonon frequencies due to light mass of B atoms. It has also been observed that the pseudo-atom model (Model-II) with appropriate choice of the potential parameter r_c can successfully explain high value of T_c and isotope effect in MgB_2, confirming the prominent role played by electron-phonon interaction in the high T_c superconductivity observed in MgB_2. The isotope effect exponent α-values obtained from the two models are in excellent agreement with each other and the present value α= 0.462 is also much closer to the BCS value of 0.5. Interaction strength N_oV-values obtained from the two models are also in excellent agreement with each other and the present value N_oV=0.407 suggests that MgB_2 is a strong coupling superconductor. The present unified approach thus successfully explains superconductivity in Mg, B and MgB_2.

Key Words : Pseudopotential, superconductivity, transition temperature, electron-phonon coupling strength, isotope effect, interaction strength.

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Electronic structure of hydrogenated diamond surfaces: The role of temperature on surface reconstruction.

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Nanocrystalline diamonds are currently widely proposed as promising [1] in the development of new devices for biosensing and bioelectrochemistry, due to its uncommon surface electronic properties such as negative electroaffinity [2], sensibility to the surface termination, and expressive reduction of resistivity [3]. Usually obtained by chemical vapor deposition in a controlled way, the surface of the samples imaged from scanning tunneling measurements [4] and atomic force microscopy [5] shows a number of complex structures due to local reconstructions, which are demonstrated to be dependent on the exposition to hydrogen, and on the temperature of the sample [4]. In this work we present a study of the electronic structure for different surface reconstructions, with local defects such as interruptions of dimer rows and dangling bonds at the surface, in order to identify the role of hydrogen atoms in the electronic properties. Due to the above mentioned role of temperature and hydrogen exposition on the surface termination, in order to describe theoretically these specificities it is necessary to take into account, in the theoretical modeling, the dynamics under finite temperatures, with larger unit cells than those currently accessible to the treatment under first principles theory. Hence, to this end we use semi-empirical tight binding molecular dynamics to generate models [6], which are then studied in depth through density functional theory [7,8].

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Main Topic: A7 Spectroscopies

The nonempirical calculations of the lattice dynamics of the oxyfluoride Rb_2KTiOF_5

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The elpasolit Rb_2KTiOF_5 undergoes at 215 K a structural transition Fm3m (Z=4) <->I4/m (Z=10). The structural distortion is due to rotation of all octahedral around the four-order axis through an angle of about 3°, a distortion of some octahedra, and the significant displacements of some Rb atoms. When refining the structure, it was impossible to recognize oxygen and fluorine atoms. The studies of the structure and Raman spectra of the cubic phase of Rb_2KTiOF_5 showed that disordering take place at least in the octahedral subsystem.

In this study we calculate phonon dispersions, Born effective charge, high-frequency permittivity of the Rb_2KTiOF_5 of several ordered configurations. The dynamic properties are calculated using a nonparametric generalized Gordon-Kim model in which the deformability, dipole and quadrupole polarizabilities of ions are taken into account.

The $TiOF_5$ anion exhibits tetragonal symmetry C_{4v}. However, symmetry of the crystal lattice oxyfluorides remains cubic with space group Fm3m due to statistical disorder of F and O atoms. We calculated the vibration frequencies of atoms in the compounds of several ordered configuration. In the first configuration there is only one orientation of the octahedra in the Fm3m unit sell (F-Ti-O along +z), in the second ordered configuration there are two nonequivalent octahedra in the Fm3m unit sell (F-Ti-O along +z and –z) and in the third configuration there are four nonequivalent octahedra in the Fm3m unit sell (F-Ti-O along +z and –z). Frequency spectrums of these ordered configurations are consisting “soft” lattice modes; it means, that studying ordered configurations undergoes a phase transitions.

The eigenvectors of both “soft” lattice modes of first configuration correspond to the equivalent displacement of all Rb atoms and the rotation of all the octahedra. There are “soft” lattice modes in the second and third configurations which the eigenvectors correspond to the nonequivalent displacement of Rb atoms, the rotation of the some octahedra and the distortion of the some octahedra. Also, there are some lattice modes of relatives on frequency to the highest in the second and third configurations. Raman spectra of the cubic phase of Rb_2KTiOF_5 showed that disordering take place. The phase transitions can be attributed to instability one of a “soft” lattice mode in the second or third configurations.

Main Topic: A1 Nanoscience

Pseudo-electromagnetism in graphene

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We present roles of pseudo vector and scalar potential in changing physical properties of graphene systems. First, graphene under small uniaxial strain is shown to be described by the generalized Weyl's Hamiltonian with inclusion of pseudo vector and scalar potential simultaneously [1]. Thus, strained graphene is predicted to exhibit velocity anisotropy as well as work function enhancement without any gap. Second, if homogeneous strains with different strengths are applied to each layer of bilayer graphene, transverse electric fields across the two layers can be generated without any external electronic sources, thereby opening an energy gap [2]. This phenomenon is made possible by generation of inequivalent pseudo scalar potentials in the two graphene layers. Third, when very tiny lateral interlayer shift occurs in bilayer graphene, the Fermi surfaces of the system are shown to undergo Lifshitz transition [3]. We will show that this unexpected hypersensitive electronic topological transition is caused by a unique interplay between the effective non-Abelian vector potential generated by sliding motions and Berry's phases associated with massless Dirac electrons.

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Main Topic: T1 Density-Functional Theory beyond LDA

PAW method in localized-basis-set SIESTA code: first stage of development

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The Projector Augmented Wave Method (PAW) has been demonstrated to be a particularly efficient and accurate tool to perform electronic structure calculations. The main advantage of this method is that it has a computational cost similar to that of a pseudo-potential calculation while retaining the key physics of all electron methods, including the correct nodal behavior of the valence electron wave functions and an easier inclusion of the upper core electrons in the self-consistent cycle.

The SIESTA code uses a linear combination of pseudo-atomic orbitals as a basis set, and in the present form of the code, the calculations are made within the formalism of Norm-Conserving Pseudo-Potentials of the Troullier-Martins type in their fully non-local form.

In some magnetic systems, for example Fe-based alloys, there is an expected improve of accuracy on the calculations of their properties with the PAW method as has been reported in the literature. Several publications show that values calculated with the PAW method compare very well with more accurate full-potential calculations. The motivation for the implementation of this method on SIESTA is to combine the higher accuracy of the PAW method and the more efficient basis set.

Main Topic: T9 Response to External Fields

A simulated reflectivity experiment: theoretical optical spectrum of strained-lattice bulk $SrTiO_3$

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Reflectivity and absorption measurements are powerful techniques to investigate microscopic properties of matter. Among these properties, modifications in the lattice structure of a system can be detected via differences between measured signals. Nevertheless a simple interpretation of measured data is difficult to give since the absorption of incoming photons gives rise to a vast variety of phenomena that are collectively described by the macroscopic dielectric tensor of the sample.

Near the optical gap of many semiconductors and insulators, the principal contribution to the dielectric tensor is given by the electrons of the solid absorbing the light and by their collective response. In this scheme, a theoretical dielectric response obtained in the framework of independent particles is not accurate enough to reproduce experimental data. Because of this, more advanced techniques are mandatory, especially because of the inclusion of collective reactions as screening and electron-hole interactions.

Here we present a theoretical study carried on the optical properties of bulk S rT iO_3 (STO) with two different lattice structures : one is the cubic structure (a = 3.905 Angstrom[1]) and one is a strained configuration. We present the computation of the macroscopic dielectric tensor of STO performed in the framework of Time Dependent Density Functional Theory (TDDFT), where the exchange-correlation kernel has been approximated using either the Random Phase approximation (RPA) or the Long Range Contribution kernel (LRC)[2]. To improve the calcu- lation of the band structure, Many Body Perturbation Theory (MBPT) has been applied in the LDA+G_0 W_0 approach, suggesting the use of a scissor operator to account for the scree- ning. Bethe-Salpeter Equations has been finally solved for the cubic structure to improve the description of the excitonic effect. Comparison with experimental data[34] has been also carried out.

Using a C++ code[5] written ad hoc to compute the reflectivity of anisotropic materials, we will display the difference in signal due to the structural strain and we will link it to the difference between the two theoretical dielectric tensors.

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Main Topic: T1 Density-Functional Theory beyond LDA

Ab initio study of electronic properties of bismuth

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Bismuth, a group-V element which crystallizes in the rhombohedral A7 structure, is a well-known semimetal, and the archetype of thermoelectric materials. Our purpose is to interpret a behavior of the plasma frequency with respect to the pumb/probe delay in photoexcited bismuth. The from-first-principles calculations are performed in the framework of the density functional theory with the generalized gradient approximation, using a plane wave basis set and pseudopotential scheme. Satisfactory agreement with reported experimental results have been obtained. In particular, we show that the role of spin-orbit coupling effect has been found to be crucial to satisfactory obtain both the electron and hole pockets at the Fermi level.

Applications: A5 Functional Materials

Numerical simulation of four-probe resistance measurements of nanoscale materials

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Four probe measurements are widely used to measure the intrinsic resistance of a sample without the contact resistance at interfaces between the sample and source/drain electrodes. However, the four-probe measurements of nanoscale materials often fail to capture the intrinsic resistance of the samples when the distance between probes is shorter than the phase relaxation length of the sample. To clarify the relation between the intrinsic resistance of sample and data of four-probe measurements at nanoscale, we have developed a four-probe electron transport simulator using the nonequlibrium Green's function method combined with the self-consistent-charge density-functional tight-binding method. In the present work, we have carried out the four-probe resistance calculation of individual single-walled carbon nanotubes (SWNTs).
The two simulation models we adopted are depicted in Fig. 1(a). We used (5, 5)-SWNTs as both a sample and probes. For both the models, we observed the appearance of sharp peaks and dips in four-probe resistance ($R_{4\mathrm{pt}}$) spectra as depicted in Fig. 1(b), which is not expected in measurements on macroscale pristine sample without defects. In order to clarify the origins of the sharp peaks and dips, we have calculated DOS of the sample and LDOS at the apex of a current probe in model A, which are also shown in Fig. 1(b). We can see that the peaks and dips in the four-probe resistance spectra correspond to peaks in either the LDOS or DOS. The results suggest that in this regime the effects of current probes in four-probe measurements are not completely removed and the features of the sample appear in a way different from macroscopic measurements.

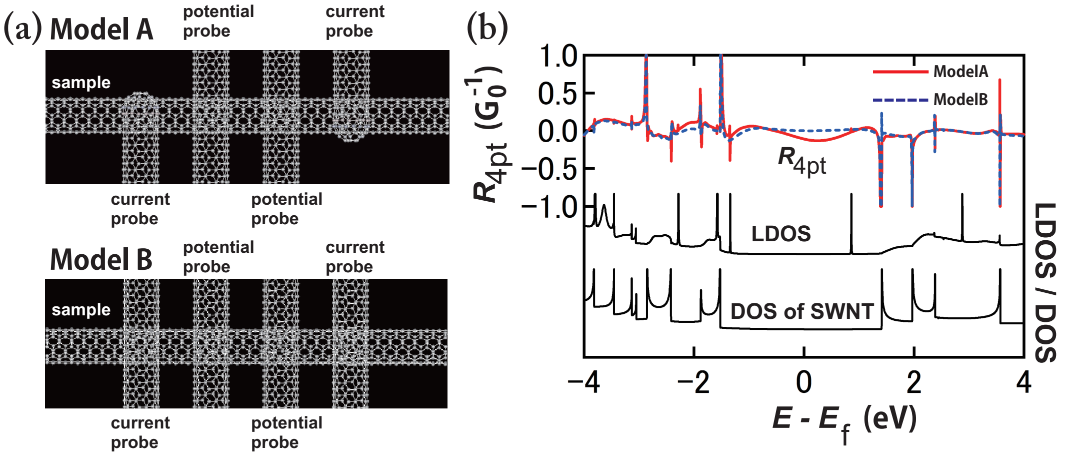

Figure 1: (a) Schematics of the simulation models. Both model A and model B consist of a sample, two potential probes, and two current probes, all of which are (5, 5)-SWNTs. The apices of current probes contact the sample in model A, while the current probes and the sample cross in model B. (b) Four probe resistances of the models, LDOS at the apex of a current probe in model A, and DOS of SWNTs.

Main Topic: A7 Spectroscopies

Characterization of point defects in UO_2 by positron annihilation spectroscopy: a first-principles study

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Positron Annihilation Spectroscopy (PAS) is one of the most powerful experimental tools for probing defects in crystalline materials. Its great sensitivity to vacancy-type defects is due to the fact they act as efficient positron traps because of the reduced repulsion of positive ions. However, the correct identification of defects with PAS requires the knowledge of accurate positron lifetimes for the various kinds of defects. That can be provided by numerical calculations.

The interpretation of PAS experiments calls for theoretical methods with quantitative predicting power. Such a method must accurately treat on the same footing, the electrons and positron densities as well as the atomic structure. The TC-DFT[1,2] (Two-Component Density-Functional Theory) has proven its capability to answer this problem. We have implemented this formalism within the "Projector Augmented-Wave" (PAW)[3] method in the ABINIT code[4]. In our implementation, the electrons and positron densities are optimized self-consistently and positron-induced forces are accurately calculated. That allows to properly determining the relaxed geometries of defects that trapped positron.

In this work, we have applied the TC-DFT to various point defects in UO_2. The use of the PAW method allows considering large super cells to simulate point defects, we have typically used cells that contain 32 UO_2 unit formulas (t96 atoms). Uranium dioxide is well known to be poorly described by standard DFT because of strong electronic correlations. We chose to use the LDA+U framework in order to overcome this shortcoming.

Various kinds of defects have then been investigated: the oxygen vacancy, the oxygen interstitial, the uranium vacancy, and three Schottky defects. This work is a first attempt to help for the interpretation of PAS experiments on UO_2 but it seems really promising. In particular, we have demonstrated that the TC-DFT could be successively applied for treating strongly-correlated materials like UO_2 if the Hubbard correction is included.

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Main Topic: T8 Electronic Transport

Electron-phonon coupling in semiconducting nanostructures

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Interaction of excited electrons with phonons plays a central role for electronic and transport properties on the nanoscale. It is the main process limiting the excitation lifetime at values of energy around 0.5 eV above the bottom of the conduction band.

Recently, we have developed a theoretical approach, fully ab initio, which allows us to calculate the electron-phonon coupling constants and scattering times for collisions of charge carriers in the conduction band with short-wavelength phonons [1,2]. This approach is based on the density functional theory [3,4], and has enabled us to describe the relaxation of hot electrons in GaAs, and to calculate the lifetime of the direct exciton in GaP, all in complete agreement with experiments. We have also described the evolution of the lifetime of the direct exciton in GaAs under pressure[5], which is governed by the electron-phonon scattering rate.

We will also present our new results about the intrinsic lifetime limit of the $2p_0$ shallow impurity state in silicon doped with group V donors, especially phosphorous [6]. Lastly, the effect of the nanostructuring on the electron-phonon coupling constant will be illustrated through the example of GaAs/AlAs superlattices. Our results show that the electron-phonon coupling constants in those layered materials are widely different from the bulk ones.

We would also like to point out that such an approach to compute the electron-phonon coupling is crucial to tackle the coupling of the charge and heat transports in nanostructures. We will present results of the electronic mobility in silicon computed with ab initio deformation potentials for the intervalley scattering and the Boltzman equation[7].

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Main Topic: A1 Nanoscience

The absorption of diamondoids from time-dependent density functional calculations

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Recent technological developments allow the size and shape selected preparation of small diamond nanocrystals, i.e. diamondoids [1], that are the smallest building blocks of diamond. Since the characteristic size of these diamondoids is in the range of nanometer, they possess several interesting properties that do not show up in the case of bulk diamond. Recently, Lasse et al. measured the absorption spectrum of several pieces of the diamondoid series [2]. We show that all-electron time-dependent DFT (TD-DFT) calculations including hybrid functional in the TD-DFT kernel are able to provide quantitatively accurate results [3]. Our calculations demonstrate that Rydberg transitions are characteristic even for relatively large nanodiamonds resulting in low optical gaps. Continuing our work on pristine diamondoids [3], we also investigate how impurities may affect the optical properties of small diamondoids.

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Ab initio prediction of giant magnetoelectric effects driven by structural softness

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

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

We demonstrate this notion with calculations for thin films of room-temperature multiferroic $BiFeO_3$. We show that under certain epitaxial conditions these films display a linear ME response comparable to the largest ones ever measured.

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Main Topic: T2 Time Dependent DFT

A DFT/TDDFT study of di-zinc pyrazinoporphyrazine-phthalocyanine complexes with different peripheral substituents as potential sensitizers in a DSC

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We performed a theoretical study of the electronic structure and the characterization of the electronic transitions in the UV-vis absorption spectra of a family of dimers constituted by Zn(II)-Pyrazinoporphyrazine and Zn(II)-Phthalocyanine linked by pyrrolic rings through =CH- group, with peripheral electron-donors and electron-withdrawing substituents R (Fig. 1) (**1.** OH, **2.** $C(CH_3)_3$[1], **3.** CH_3, **4.** Phenyl, **5.** H, **6.** CO_2H, **7.** CN, **8.** NO_2 and **9.** PO_3H_2) via relativistic two components ZORA Hamiltonian using Density Functional Theory (DFT) and its extention Time Dependent-Density Functional Theory (TDDFT). The geometries were optimized using the Generalized Gradient Approximation, BP86 functional, and Slater Type Orbitals (STO-TZP) basis set, using the ADF computational package[2].

These complexes are excellent chromophores and they show interesting molecular properties like being useful for redox catalysis, photocatalysis and for building optical devices. That is why these results prompted us to do a proposal to study which substituent R will increase the light-harvesting capability of the different systems in a dye-sensitized solar cells (DSC) device with possible injection to the semiconductor (Figure 1).

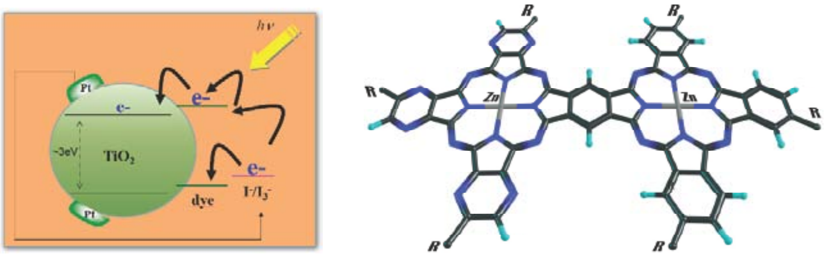

Figure 1. DSC mechanism and general molecular structure of the studied systems.

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Main Topic: T2 Time Dependent DFT

A theoretical study of the effect of the bridge (=CH-, =N-, -O-, -S-) connecting di-Zinc pyrazinoporphyrazine-phthalocyanine complexes

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Experimental and theoretical studies show a variety of porphyrazine complexes with metallic center like Ti, Ni and Zn, forming diverse types of dimers or trimers[1]. These type of complexes are considered excellent sensitizers in the design of dye-sensitized solar cells obtaining an efficient photocurrent generation. The aggregation is avoided when the dye is anchored to a semiconductor film through generally the carboxylic acid group, mainly by the inclusion of the *tert*-butyl substituents in the ring[2,3]. Also an important aspect is the charge separation; this can be analyzed through the compositions of the frontier molecular orbitals, where the HOMO is localized in the donor subunit and the LUMO over the acceptor subunit[3]. Today, there is a search of a sensitizer that achieves effective absorption of sunlight in the red and near-IR region, to transform these photons into electricity, for this reason we performed a theoretical study of the electronic structure, the orbital composition and the characterization of the electronic transitions in the UV-vis absorption spectra of a family of dizinc pyrazinoporphyrazine-phthalocyanine compounds linked by pyrrolic rings through of the =CH-, =N-, -O-, -S- (B in Fig 1) motifs, via relativistic two components ZORA Hamiltonian using Density Functional Theory (DFT) and its extention Time Dependent-Density Functional Theory (TDDFT). The geometries were optimized using the Generalized Gradient Approximation, BP86 functional and Slater Type Orbitals (STO-TZP) basis set. All calculations were carried out using the ADF computational package[4]. The study are guided to determinate the effect in the electronic structure and in the optical properties of this family of dimers.

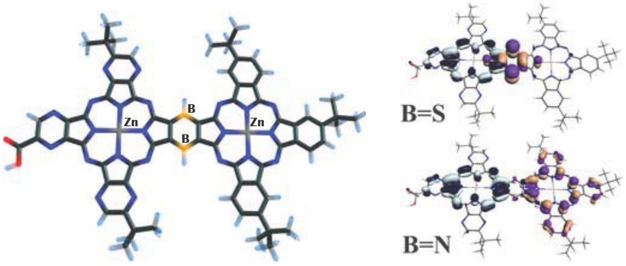

Fig 1. Molecular structure diagram and frontier molecular orbitals for the complexes with B=S,N.

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Main Topic: T2 Time Dependent DFT

Optical properties and aromaticity of meso substituted porphyrins

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The porphyrine macrocycles are well known because of its use as supramolecular bulding block and also its new use as solar cell sensitizers. The ring substitution in the *meso* position and in the pyrrolic ring that form the macrocycle, changes and modulates the properties of these systems, like the redox chemistry, shifts the absorption bands in the UV-Vis spectra, and so on. We studied both systems, substituted in the meso position by phenyl and hydrogen, but also, substituting the H in the pyrrolic ring by halides, see Figure 1. In order to get a better description of all the known characteristics of these macrocycles we have taking into account the Spin-Orbit effect by using ZORA Hamiltonian, that includes the scalar and also the Spin-Orbit corrections. We also calculated absorption spectra using the TD-DFT formalism, the IR frequencies and the NICS (nuclear independent chemical shift) indexes (in several points of the rings) observing the influence of the substituent over the aromaticity and the importance of the Spin-Orbit correction in all these measurements.

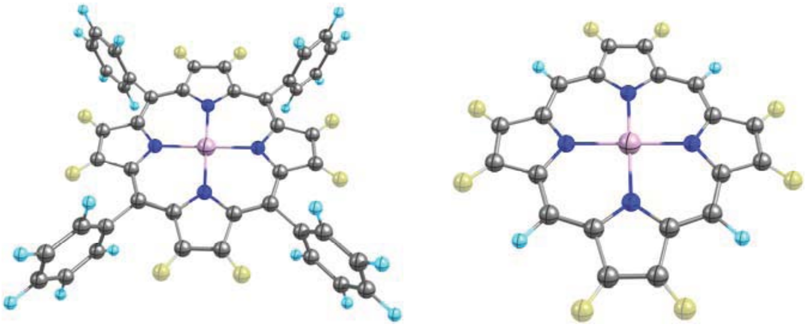

Figure 1: Studied Porphyrin substitued in the meso position with hydrogen and phenyl ring. In light yellow are shown the position of the different changed halide atoms.

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The role of van der Waals forces in semiconductor solids

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While the importance of van der Waals forces (vdW) for binding between molecules is well established, their influence on the cohesive properties of solids remains to be quantified from first-principles. In particular, most state-of-the-art (semi-)local density functionals yield systematic deviations for the lattice constants, cohesive energies, bulk moduli and their pressure derivatives for a range of solid-state systems. The traditional way to calculate vdW dispersion coefficients in solids is to obtain the polarizability from the dielectric function by means of the Clausius-Mossotti equation. Here, we assess the validity of the Clausius-Mossotti equation for semiconductor solids. We evaluate the long-range C_6 dispersion coefficients for diamond, Si, and Ge from the TDDFT dielectric function as well as by using the cluster extrapolation model. We find good agreement between these two different approaches, enabling us to assess the effect of the long-range vdW forces on the abovementioned cohesive properties. In particular, for Si and Ge, we obtain improved results by coupling the long-range dispersion energy with the Perdew-Burke-Ernzerhof (PBE) functional for the short range. We compare our results for the cohesive properties with recently developed functionals for solids.