POSTER SESSION II

FRIDAY 11 JANUARY 2013

In alphabetical order of presenting author (underlined)

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

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A4

Dielectric Properties of Functional Oxide thin-films from First Principles

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A5

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

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A11

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

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A1

Edge functionalization of zigzag graphene nanoribbons with sodium

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A1

Layered Cobalt Oxides for Oxygen Evolution Reaction

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A8

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

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A3

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

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A5

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

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Electronic localization and magnetism in intermetallic alloys from ab initio calculations

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A3

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

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A7

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

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A7

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

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Magnetism in thiolated gold model junctions

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

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A7

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

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A6

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

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

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Density functional simulations of Sb-rich GeSbTe phase change alloys

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

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Electron-hole puddles in the absence of charged impurities

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

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

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

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Clustering and Diffusion of Hydrogen in α-Fe Including Quantum Effects

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A10

Ab Initio Study of Magnetic Anisotropy Energy of Some Low Dimensional Systems

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Substrate and chemical functionalization induced magnetic moment on hexagonal boron nitride

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Ab Initio Study of the Adsorption of NO on small Rh clusters supported on MgO

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Study of Structural, Electronic and Magnetic Properties of Pd_n, Pd_nMn_1 and Pd_nMn_2 clusters

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A3

Study of Al/Al2O3 Interface with Reactive Force Field

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A6

Electrocaloric effect in ferroelectric alloys from atomistic simulations

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A5

EELS Signature of Boron Nitride Nanoribbons

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Role of pyridine derivatives on the electronic properties of polymer/metaloxide interfaces for photovoltaics

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Study of nanoconfinement of O_2 molecules in fullerenes and nanotubes

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

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Anderson localization in crystalline phase-change materials

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

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A11

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

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

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A5

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

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

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A6

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

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Topological defect formation and activation in carbon nanostructures

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Microscopic charge fluctuations in hexagonal boron nitride

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Ideal Energy-Level Alignment at the ZnO/P3HT Photovoltaic Interface

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First-principles calculations of the structural and electronic properties of zinc blende BxIn$1-x$N

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A10

The effect of ligand adsorption on the structure of metal nanoparticles

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Scattering potentials of defects on Ge(001) surfaces

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A6

Optical properties of ordered defect compounds for $CuIn_5Se_8$ and $CuIn_3Se_5$: An ab-initio study

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A7

Calculating quasiparticle energy-level alignments at molecule/semiconductor interfaces

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Fundamental limits on transparency: first-principles calculations of absorption

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A5

Atomic-scale insight into self-segregation and diffusion processes on a Ni/Cu bimetallic surface

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A6

First principle study of donor wave functions in silicon nanowires
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The evaluation of perovskite phase transitions using AIDA, a materials informatics platform for materials design and discovery
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A10

First-Principles Study on Carbon Emission Process at 4H-SiC(0001) Surfaces and 4H-SiC(0001)/SiO2 Interfaces
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Influence of Al concentration on the opto-electronic properties of Al-doped MgO
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A7

DFT Studies on the Adsorption of Atomic Sulfur and Methanethiolate at Coinage Metal Surfaces
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A6

CHP molecule filling the pores of the h-BN/Rh(111) nanomesh: A computational study
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Electronic structure calculations on MX2 dichalcogenide/Graphene hybrid structures.
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Structural and Electronic Properties of IV Nanowires: Ab-initio Study
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Size dependent electronic properties of ZnO nanowire: Ab-initio study
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Optimal interface doping at La2/3Sr1/3MnO3/SrTiO3(001) heterojunctions for spintronic applications

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A3

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

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A6

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

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

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

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A1

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

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A11

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

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Spin crossover induced by an electric bias in nanoscale devices

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A3

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

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Main Topic: A4 Geophysics

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

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The power supplied to the geodynamo, measured by the heat-flux across the core-mantle boundary (CMB), places constraints on the evolution of Earth's deep interior. Estimates of CMB heat-flux depend on properties of iron mixtures under the extreme pressure and temperature conditions in the core, most critically on the thermal and electrical conductivities. We computethese conductivities at core conditions for liquid iron mixtures that fit the seismologically-determined core density and inner-core boundary density jump using density functional theory. We find both conductivities to be 2-3 times higher than estimates in current use. The changes are so large that core thermal histories and power requirements must be reassessed. New estimates of adiabatic heat-flux give 15-16 TW at the CMB, higher than present estimates of CMB heat-flux based on mantle convection. A thermally stratified layer beneath the CMB is therefore inevitable unless a very high present-day CMB heat-flux can be maintained, which requires a rapid CMB cooling rate and an inner core that is only ~300-400 Myr old. We estimate stable layer thicknesses using the condition of neutral buoyancy for a range of plausible values for CMB heat-flux, finding thermally stable layers that can span hundreds of kilometres. These calculations also suggest that compositional buoyancy is insufficient to overcome the large stabilising thermal gradient; any convection in the upper core must be driven by penetration or instabilities arising from convection deeper inside the core, or by lateral variations in CMB heat flow.

Main Topic: A5 Functional Materials

Dielectric Properties of Functional Oxide thin-films from First Principles

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Abstract:

Perovskite oxide materials have attracted researchers for many years because they show a wide range of physical properties that make them interesting both technologically and scientifically, e.g., ferroelectricity, superconductivity, amenability to a variety of dopant additions, etc. Particular attention has been drawn to perovskites in thin-film form in order to meet the demand of manufacturing smaller industrial components such as advanced integrated electronic devices.

The optical properties of thin-film perovskite oxides can differ significantly from those of the bulk due to several factors, such as the mismatch strain imposed by the substrate, cation substitution and arrangement, point defects, etc. We investigate the effect of some of these factors on the optical properties of functional oxide materials ($BaTiO_3$ and $SrTiO_3$). The optical properties are calculated from first principles using density-functional theory within the local density approximation (LDA).

First, it is found that the refractive index increases with applied strain, whether uni-axial or isotropic. This is observed in the visible range of spectrum (400-700 nm), and the change is almost linear. Second, the optical properties of $Ba_xSr_{1-x}TiO_3$ (BSTO) solid solutions are studied using both the supercell and the virtual-crystal approximation (VCA) approaches. It is found, surprisingly perhaps, that the two methods agree remarkably well. The underlying reason is found to be that the band transitions responsible for the visible range of spectrum (400-700 nm) are very similar in both approaches. Third, the effect of Sr content in BSTO is investigated. It is found that the refractive index varies (decreases) almost linearly as the Sr:Ba ratio increases. Finally, the effect of different atomic configurations of Sr atoms for a constant Sr:Ba ratio in BSTO is studied.

Theory and Methods:
T11 Density Functional Theory within LDA.

Applications:
A5 Functional Materials

Main Topic: A11 Other applications

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

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The mechanism of the α-ϵ transition in iron is reconsidered. A path in the Burgers description of the bcc/hcp transition different from those previously considered is proposed. It relies on the assumption that shear and shuffle are decoupled and requires some peculiar magnetic order, different from that of α and ϵ phases as found in Density-Functional Theory. Finally, we put forward an original mechanism for this transition, based on successive shuffle motion of layers, which is akin to a nucleation-propagation process rather than to some uniform motion.

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

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The growth of Ge on Si films exhibits a transition from 2D to 3D growth with formation of metastable 3D hut clusters with {105} facet structure. These clusters are characterized by perfect facet planes, which imply a nucleation barrier for the growth of a new atomic layer on the {105} facets. Depending on growth conditions, shape transition from nearly square base hut to elongated base one occurs during cluster growth. Such a transition could be described by kinetic models for the growth of Ge huts with a barrier for nucleation of each successive atomic layer on {105} facets. However, various kinetic models assume different mechanism for the new {105} facets growth, whether these facets start growing from the base of the hut or from its apex. Furthermore, there are models, which predict the hut formation by transition from tiny islands, which form with no nucleation barrier due to surface-energy anisotropy of a strained SiGe film. Hence, a detailed study of relaxed hut surface morphology may provide a better understanding of the growing mechanism, and, subsequently, a way to control the growth of Ge hut clusters. In the present work we performed an ab initio study of various nucleation sites of Ge dimers on relaxed {105} facets of a Ge hut. We have considered the case of small elongated Ge huts (≈ 3000 atoms) on SiGe film (≈ 17000 atoms). All calculations have been done by using the CONQUEST code, which is a DFT based linear scaling method. An important step of these calculations is the optimization of atomic positions. Preliminary results show that nucleation sites at the hut apex and close to the edges between {105} facets are energetically more stable.

Main Topic: A1 Nanoscience

Edge functionalization of zigzag graphene nanoribbons with sodium

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Pristine graphene is a zero-bandgap (perfect) semimetal. The conduction and valance bands of graphene meet linearly at six distinct points (Dirac-points) of first Brillouin zone, and are in the form of symmetric cone tips at the Fermi level [1]. Long and thin strips of graphene, known as graphene nanoribbons (GNR), are semiconducting and they have been experimentally realized with smooth edges [2,3]. As a special class, zigzag-edged GNRs (ZGNR) have width dependent energy band gaps, and are also expected to present edge localized spin states [4]. Modification and functionalization of ZGNR edges change their electronic structure and give the opportunity to engineer their properties. For instance, recent studies [5, 6] have shown ways to obtain half-metallic ZGNR.

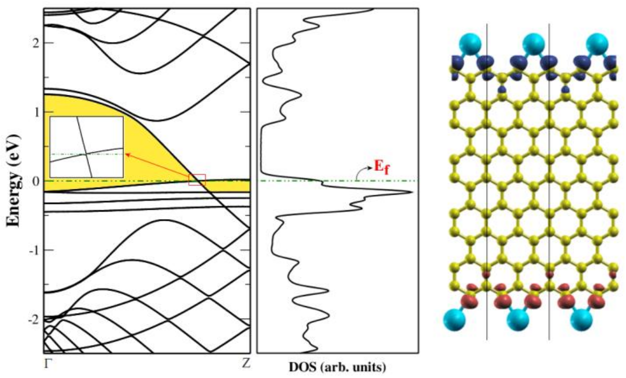

Fig. 1: Band structure and density of states diagram (left), and relaxed geometric structure and isosurfaces of charge density difference of spin-up and spin-down states (right) for Na terminated 9-ZGNR. The inset magnifies the tilted Dirac cone at the Fermi level. Positive and negative values of the charge density difference is shown by red (dark) and blue (light) regions, respectively, for the same isosurface value of ±0.0025 electrons/Å^3.

In this study we report that edge saturation of ZGNRs with Na atoms at a specific concentration makes them a zero-gap, one-dimensional semimetal with asymmetric linear energy dispersion around the Fermi level. That corresponds to a Dirac "cone" similar to pristine two dimensional (2D) graphene [1], however, with a tilted form. Also half-coverage concentration of Na terminated 9-ZGNR have same pseudospin as graphene. Similar to hydrogenization of the edges, Na atoms saturate the dangling bonds of edge carbon atoms, and modify the local magnetic moment magnitudes and change the electronic band structure. Binding of sodium atoms reduces the magnetic moments of the edge carbon atoms from $\mu = 1.21\ \mu B$ to $\mu = 0.11\ \mu B$. This magnetic moment reduction is comparable to the hydrogenation of ZGNRs where edge carbon magnetic moment $\mu = 0.26\ \mu B$ [7]. As seen in figure, there are no net induced magnetic moments on the sodium atoms, and Na transfers %10 of its total valance charge to the ribbon.

Geometry optimizations and calculations of magnetic and electric properties were performed using the SIESTA package based on density functional theory (DFT).

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Layered Cobalt Oxides for Oxygen Evolution Reaction

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Abstract: The presence of layered cobalt oxides have been recently experimentally identified in Co-based anodes under oxygen evolving conditions[1,2]. In this work, we perform theoretical investigation of surface stability and oxygen evolution activity in these systems. We consider A_xCoO_2 type compounds with four types of light alkali metals (A=H,Li,Na,K) intercalated between CoO_2 layers in three versions of oxygen stacking. All the energetics is obtained via density functional theory with the Hubbard-U correlation (GGA+U) approach , which has been demonstrated to be necessary for accurate description of bulk, surface and recently also catalytic properties of transition-metal oxides[3]. We identify oxygen covered (01-21) surface termination of β-CoOOH prototype as dominant surface under oxygen evolving conditions. Further, the obtained overpotentials for multiple structures and surface terminations all lie within 0.75 to 1.0 V range with two distinct positions on the volcano plot. The best activity is observed for (01-12) surface of α-$NaCoO_2$ with overpotential η =0.75 V. We also predict relatively large 0.29 V improvement in the theoretical overpotential for 25% Fe surface-doped α-$NaCoO_2$. Finally, I will present the calculated Co K-edge spectra calculations of above compounds and discuss their relation to recent experiments at SLAC[4].

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

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The III-VI DMS materials represent a relatively unexplored class of materials especially from a theoretical standpoint. $In_{1-x}Mn_xS$, is a new member of III-VI DMS class which has studied experimentally by G.Franzese &.all.

First principles calculations for $In_{1-x}Mn_xS$ are carried out by using full-potential linear augmented plane wave (FP-LAPW) method, based on the framework of density functional theory (DFT) as implemented in Wien2k code. The exchange-correlation potential use in these calculations is evaluated in the local spin density approximation (LSDA). The electronic structure and magnetic properties of Mn doped InS for 25% doping concentration are investigated.

For this purpose, we have considered a supercell with 16 atoms ($In_6Mn_2S_8$). It is found that this doped configuration favors the ferromagnetic ground state. In the other hand, electronic structure calculation shows that total magnetic moment for the supercell is 4 μB, which is mainly contributed by dopant Mn 3.939 μB, with a little contribution from S atoms due to the hybridization between Mn 3d and S 3p electrons. We have also showed the half-metallic ferromagnetic character of $In_{1-x}Mn_xS$ alloy, from calculated band structures for two contributions (spin-up and spin -dn) and from total and partial densities of states. The exchange constants $N_0\alpha$ and $N_0\beta$ are also determined in the mean field approximation, which are considered to be an important parameters for describing DMSs.

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

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Displacive phase transitions, in which the small cooperative displacement of atoms defining the transition are the same modes driving lattice dynamics, appear in a wide range of systems within mineral sciences, metallurgy and functional materials. One of the prototypical examples is the ferroelectric transition in several oxide perovskites, for example $BaTiO_3$, where the cooperative off-centering of the Ti ions produce a macroscopic polarization. These oxides are also commonly susceptible to other types of symmetry lowering transitions involving the rotation of the oxygen octahedra. These rotations, also known as antiferrodistortive modes, are typically thought to compete with the ferroelectric mode. Determining the competition between all possible modes and the full phase diagram of these materials is of importance for both fundamental understanding and device applications.

The development of effective Hamiltonian approaches, which attempt to capture the energy landscape of the lowest energy modes derived from density functional theory [1,2], made the first principles study of lattice dynamical phenomena practically possible for the first time and has already been successfully applied to several bulk oxide crystals. However by neglecting all but the lowest frequency modes, this scheme is likely inadequate to tackle more complex cases involving several competing distortions or where the relevant degrees of freedom are *a priori* unknown. In an attempt to overcome these limitations, we present the application of a new approach based on the effective Hamiltonian scheme but now including all the phonon modes, not only the lowest frequency ones (for details see J. Wojdel's poster). We will present work in progress on building and applying the all-atom first principles effective Hamiltonian to oxide perovskite superlattices of $SrTiO_3$ and $PbTiO_3$ which has been suggested to display improper ferroelectricity [3] involving the coupling of ferroelectric and antiferrodistortive modes.

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

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Metal-oxide nanoparticles (especially TiO2, ZnO, SnO2) may be sensitized to harvest visible radiation in working solar cells, upon proper functionalization. However, at present the principles regulating interactions between the oxide layer and the rest of the photovoltaic (PV) cell are poorly understood. Indeed, upon sensitization with molecular and/or inorganic layers, semiconductor surface interacts in a wide range of possible scenarios, driving the formation of interfaces with specific spatial arrangement and novel electronic properties, and affecting both the light harvesting and the generation of the photovoltaic current.

By means of ab initio DFT calculations, we characterize the optoelectronic and transport properties of the main subsystems that form the active layer of a prototypical PV solar cell, based ZnO. We will consider both hybrid organic/ZnO and fully inorganic heterostructures.

Firstly, we report on the functionalization of the non-polar ZnO(10-10) surface upon the adsorption of prototypical chromophore linkers, such as catechol cyanin dyes also in the presence of water solvent [1-2]. Then, we consider the metal/semiconductor interface between ZnO and Al layer, that are representative of the formation of the contacts with the external leads, for the collection of the photocharge. Particularly crucial is the early stage deposition of the Al layers on the polar ZnO(0001) surface [3], because of the presence of internal polarization fields in the ZnO part on one hand, and of the strong doping behaviour of Al on the other hand [4].

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Electronic localization and magnetism in intermetallic alloys from ab initio calculations

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In Ni_2MnGa, the prototype representative of magnetic Heusler alloys, the relative stability of austenite (cubic) and non-modulated martensite (tetragonal) phases depend critically on magnetic interactions between Mn atoms. While standard approximate DFT functionals stabilize the latter phase, a more accurate treatment of electronic localization and magnetism obtained with DFT+U suppresses the non-modulated tetragonal structure for the stoichiometric compound, in better agreement with the experiments. This observation can be explained using the Anderson impurity model, with Ga *p* and Ni *d* conduction electrons mediating RKKY type magnetic interactions between Mn *d* electrons. Using this picture we show that the structural properties of the material are determined by the competition between super-exchange interactions through Ni *d* and Ga *p* states. Finally, we show that off-stoichiometric compositions with excess Mn promote transition to a non-modulated tetragonal structure, in agreement with experiments.

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

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We compare the performances of the Wu and Cohen (WC, Phys. Rev. B **73**, 235116 (2006)) and of the PBEsol (Phys. Rev. Lett. **100**, 136406 (2008)) exchange and correlation functionals on the phonon dispersions of face centered cubic metals copper, silver, gold, nickel, palladium, platinum, rhodium, and iridium. The WC and the PBEsol frequencies are found to be close to each other and intermediate between the local density approximation (LDA) and the PBE (Phys. Rev. Lett. **77**, 3865 (1996)). In copper, silver, palladium, platinum, and rhodium the WC and PBEsol frequencies match the experimental inelastic neutron scattering data better than LDA or PBE. In nickel, gold, and iridium, PBE (for nickel) or LDA (for gold and iridium) remain the best functionals among these four possibilities. Calculations are performed within Density Functional Perturbation Theory extended to the scalar relativistic Projector Augmented-Wave (PAW) method. For gold and iridium we show also fully relativistic results obtained with ultrasoft pseudopotentials.

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

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October 10, 2012

1 Abstract

The phonon dispersions of different allotropic structures of iron are first calculated using the widely used embedded atom potential of Mendelev *et al.* Mendelev03 [1]. Both the low temperature bcc phase (ferromagnetic α-phase up to 1043 K, and paramagnetic β-phase up to 1184 K) and the higher temperature fcc paramagnetic γ-phase (between 1184 K and 1670 K) are considered and compared to experimental results.

This approach highlights the limited accuracy of this well known reference potential in treating vibrations at high temperature, while displaying relatively good values for the thermal expansion and elastic properties of the different solid phases. A comparison with first-principles data in the ferromagnetic and paramagnetic regime would be of paramount interest to develop more accuarate potentials. For this, we perform phonon calculations within density-functional perturbation theory on top of a spin-averaged ensemble of collinear quasi-random spin configurations, following the approach pioneered by Neugabuer and collaborators [2] to account for disorder effects and magnetic entropy.

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Catalytic Reduction of SO_2 by CO over $Pt_lAu_m(CO)_n$: A First-principles Investigation

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Sulfur dioxide is one of the main components generating acid rain, acidifying soil, and causing other forms of air pollution. Desulfurization of these combustion exhaust gases through throw-away processes are still high cost and exists disposal problem. From a practical point view, the use of CO as a reducing agent is more attractive because CO is often contained in combustion exhausts. Platinum-based material is one of the most efficient catalysts for many important processes, such as CO oxidation, and methanol dehydrogenation. However, the pure platinum catalysts are expensive, unstable, and sulfur sensitive. Bimetallic clusters often show novel properties, not presenting on either of the parent metallic clusters, and thus offer the opportunity to obtain new catalysts with enhanced selectivity, activity and stability. It is proposed that the platinum catalysts alloyed or modified by transition metals, such as ruthenium, molybdenum, and palladium, have exhibited higher activity for CO oxidation. To our knowledge, no study so far has involved the reduction of SO_2 by CO over platinum-gold bimetallic catalyst, neither in *ab initio* calculations nor experiment. In this paper, using the *ab initio* calculations, we investigate the catalytic properties of three kinds of diatomic clusters (Pt_2, Au_2 and PtAu) without and with CO pre-absorption in the instance of reduction of SO_2 by CO to COS, which can be used as agricultural fumigant. We find that, with 3 CO molecules pre-absorption, bimetallic diatomic cluster PtAu can effectively avoid catalyst sulfur poisoning. Based on our results, an ideal configurations of the bimetallic catalysts is proposed, expecting to provide a useful clue to synthesize the most suitable catalysts for purifying air pollution.

Magnetism in Thiolated Gold Model Junctions

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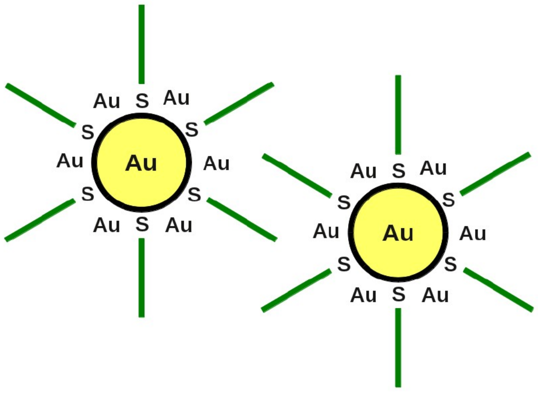
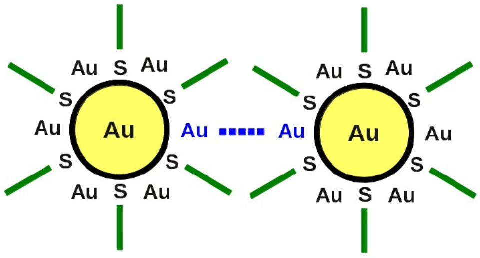
Three neutral diradical model molecules, based on pairs of small thiolated Au clusters connected via direct Au-Au bonding, are studied within the broken symmetry unrestricted density functional theory involving a set of exchange-correlation functionals, PBE, M06L, TPSS, B3LYP, M06 and TPSSh. The model systems revealing **unexpected spin-symmetry breaking** and anti-ferromagnetic spin alignment in the ground-state, within the theory used, are analyzed in terms of the total energy, HOMO-LUMO gap, vertical spin-flip energy splitting, total spin expectation values, Heisenberg exchange coupling constant J, magnetic orbitals and their overlap, diradical character, binding energies, natural bond order analysis and bond index of the central Au-Au bond. The dimers are found to be **stabilized**, w.r.t. corresponding isolated monomers, **by** the **attractive metallophilic d-d bonding**. The observed magnetism is attributed to the doublet open-shell nature of the constituents and the structural feature of the facing S-Au-S motifs in combination with the d-d interaction of the incident Au atoms, allowing a weak coupling of the spins localized sideways. The modeling provides insight to Au(I)-Au(I) interactions potentially useful in design of novel gold-based magnetic nanoscopic assemblies.





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

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Although the harmonic approximation is in many cases enough to accurately describe vibrational properties of solids, it sometimes breaks down. Whenever the dynamical behavior of the solid is not determined by the second derivatives of the potential at equilibrium but by higher order terms, the harmonic approximation may lead not only to wrong numerical values for the phonon frequencies and the free energy, but to a misleading interpretation of the stability of the system. For instance, a structure might show imaginary phonons in the harmonic approximation but might be perfectly stable due to anharmonic stabilization. In these last cases anharmonicity needs to be taken into account in the dynamical description of the solid beyond perturbation theory. We propose that the self-consistent harmonic approximation (SCHA) is the appropriate framework to tackle these problems as it seeks the physically well-defined Gibbs-Bogoliubov inequality and allows us to define the anharmonic problem through a variational procedure.

We apply the SCHA to the high-pressure simple cubic phase of calcium that is unstable in the harmonic approximation but is found experimentally. The SCHA has been applied fully ab initio including all coefficients in the dynamical potential up to fourth order. According to our results [1], the anharmonic phonon spectrum is stable and, therefore, we can state that anharmonicity stabilizes this phase. Moreover, our phonon spectrum allow us to estimate the superconducting transition temperature in this system and we found a good agreement with experimental results.

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Charge Localization Dynamics Induced by Oxygen Vacancies on the TiO_2(110) Surface and Titania and Gold-promoted Titania Surfaces

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We use ab initio molecular dynamics to investigate the dynamics of an F–center created by an oxygen vacancy on the TiO_2(110) rutile surface. The simulations uncover a truly complex, time-dependent behavior of fluctu ating electron localization topologies in the vicinity of the oxygen vacancy. Although the two excess electr ons are found to populate preferentially the second subsurface layer, they occasionally visit surface sites and also the third subsurface layer. This dynamical behavior of the excess charge explains hitherto conflict ing interpretations of both theoretical findings and experimental data. We then study the interaction of CO, H, and H_2O with the (110) TiO_2 and the Au supported (110) TiO_2 surface catalysts. The structural, electroni c, dynamical and thermodynamic properties of the titania and gold promoted titania surfaces are investigated by means of density functional theory calculations that account for the on site Coulomb interaction via the inclusion of a Hubbard term (GGA+U). The interaction between gold and substrate is accompained by an extens ive charge reorganization at the metal-oxide contact wich leads to Au oxidation and the reduction of the tit anum dioxide substrate. It is shown that the catalytic activity of the (110) TiO2 substrate is efficiently i mproved by supported and dispersed Au adatoms on the same substrate.

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

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Solid-state semiconductor-sensitized solar cells (SS-SSC) are an evolution of the concept of dye-sensitized solar cells whereby the dye sensitizer is replaced by a semiconductor quantum dot or a semiconducting nanosheet. SS-SSC have the key advantages that the expensive inorganic dye sensitizers are replaced by inexpensive semiconductor nanoparticles, and that the optical and electronic properties of the sensitizer can be tuned by exploiting quantum size effects. During the past two years SS-SSC cells have been fabricated using stibnite (Sb_2S_3) nanoparticles as sensitizers on anatase TiO_2 [1-3]. Stibnite is promising for photovoltaic applications due to its direct band gap of 1.7 eV. However this value is slightly off the ideal Shockley-Queisser gap of 1.1 eV. In order to identify semiconductor sensitizers with band gaps closer to the optimal Shockley-Queisser value, we calculated the GW quasiparticle band gaps of four isostructural compounds A_2B_3 (A=Sb,B and B=S,Se) belonging to the stibnite family. Our calculations indicate that the band gaps of stibnite Sb_2S_3, antimonselite Sb_2Se_3, bismuthinite Bi_2S_3, and guanajuatite Bi_2Se_3 are 1.6 eV, 1.3 eV, 1.7 eV, and 1.2 eV, respectively. These results suggests that antimonselite should be a promising candidate for use as semiconductor sensitizer in SS-SSC. We also discuss the sensitivity of the quasiparticle corrections to the lattice parameters and to the description of semicore states.

Work supported by the ERC under the EU FP7/ERC Grant No. 239578.

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

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The spin polarization of the emitted electrons from 3d impurities in simple metal hosts in a core-valence-valence Auger process is analyzed in terms of a first-principles density-functional theory approach, by using the golden rule. The relationship between the spin-dependent local density of states, the magnetic moments of the 3d atoms and the energy-dependent and total spin polarization of the Auger electrons is discussed. It is shown how to estimate the magnetic moment of the impurities from a measure of the total spin polarization of the Auger electrons. This can be achieved considering (i) that the Auger signal is simply due to the impurities only, (ii) the very locality of the Auger phenomenon, and (iii) a simple and general relationship between the spin polarization and the magnetic moment of the impurity which we show to be independent of the metal host. [1]
Spin selectivity in angle-resolved Auger photoelectron coincidence spectroscopy (AR-APECS) is used to probe electron correlation in ferromagnetic thin films measured by the RUs of RomaTre and Trieste. In particular, exploiting the AR-APECS capability to discriminate Auger electron emission events characterized by valence hole pairs created either in the high or in the low total spin state, a strong correlation effect in the MVV Auger lineshape of Fe/Cu(001) thin films was detected. Theoretical simulations allow one to ascribe this effect to interactions within the majority spin sub band. Such an assignment follows from a close comparison of the experimental AR-APECS lineshapes with the predictions of a model based on spin polarized density functional theory and the Cini-Sawatzky approach. [2]

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Density functional simulations of Sb-rich GeSbTe phase change alloys

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Phase change materials are of great technological importance in the realization of optical data storage devices (DVDs) and electronic non-volatile memories of new concept, the Phase Change Memory cell (PCM). Phase change materials are typically Te-based alloys and present a fast (50 ns) and reversible change between the crystalline and the amorphous phases. These two states show a large difference in the optical and electronic properties and in particular the change in resistance by three orders of magnitude across the two phases is exploited in PCMs. Presently, the alloy used as active layer in PCM is the $Ge_2Sb_2Te_5$ alloy (GST), but its low crystallization temperature prevents its use in high temperature applications (e. g. automotive applications) which require a better stability of the amorphous phase above 125 °C. In this respect it has been shown that the crystallization temperature of GeSbTe alloys raises by increasing the Sb content with respect to the stoichiometric composition $Ge_2Sb_2Te_5$. In this work we performed MD simulations of GeSbTe alloys aiming at establishing correlations between the structure of the amorphous phase and the composition. We considered the two compositions $Ge_1Sb_1Te_1$ and $Ge_2Sb_4Te_5$ [1]. The amorphous models were generated by quenching from the melt within density functional molecular dynamics. Comparison with previous results on the most studied $Ge_2Sb_2Te_5$ [2] allowed us to draw some conclusions on the dependence of the structural properties of the amorphous phase on the alloy composition. Vibrational and electronic properties were also scrutinized. Phonons at high frequencies above 200 cm^{-1} are localized in tetrahedra around Ge atoms in Sb-rich compounds as well as in $Ge_2Sb_2Te_5$. All compounds are semiconducting in the amorphous phase, with a band gap in the range 0.7-1.0 eV.

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

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Plane Wave - PseudoPotential (PP) electronic structure calculations in the Density Functional Theory framework have been successfully employed in predicting the properties of new and existing materials as well as gaining fundamental insight in quantum physics and chemistry. Due to this demonstrated success, an ever increasing number of scientists, not specifically trained in electronic structure methods, have shown interest in using the available codes in their research, often for exotic materials and systems for which available PP are limited and/or poorly tested. Moreover, applications that involve automatized massive computations in a combinatorial-chemistry perspective have also been getting more and more popular with the increasing computational power. Such calculations too, require accurate PP for a wide range of elements in the periodic table. For these reasons, a library of well tested and reliable PP is a timely necessity for electronic structure codes.

In this study, we present our efforts towards such a PP library: As a first step we have been constructing a reference all-electron data set which includes lattice constants, bulk moduli, and total energy differences of the simple cubic, face centered cubic, and body centered cubic structures of alkaline metals, alkaline earths, and transition metals. We then demonstrate how this reference all-electron data set is used to monitor and improve the performance of a library of Projector Augmented Wave (PAW) PPs (see http://qe-forge.org/gf/project/pslibrary/). Moreover, we will also report on the performance of this PP library using Quantum ESPRESSO package, in comparison with the all-electron (WIEN2K) and another PP library (VASP) for the ground state structures of a wide range of elements reported in a recent preprint [K. Lejaeghere, V. Van Speybroeck, G. Van Oost, and S. Cottenier, arXiv:1204.2733]

Electron-hole puddles in the absence of charged impurities

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It is widely believed that carrier-density inhomogeneities ("electron-hole puddles") in single-layer graphene on a substrate like quartz are due to charged impurities located close to the graphene sheet. In this poster we demonstrate by using a Kohn-Sham-Dirac density-functional scheme that corrugations in a *real* sample are sufficient to determine electron-hole puddles on length scales that are larger than the spatial resolution of state-of-the-art scanning tunneling microscopy.

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

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The adsorption of organic molecules on metal surface has attracted much attention due to their promising potential applications in organic-based electronic devices. We have studied the adsorption of pentacene molecule on the palladium Pd(100) surface, focusing on the interaction between the organic molecule and metal surface and on the alignment of molecular levels at the interface. All the calculations were performed within the framework of density functional theory (DFT) using a plane-wave basis set with ultra-soft pseudopotential, as implemented in the Vienna abinitio simulation package (VASP). The adsorption of pentacene molecule on Pd(100) surface shows flat lying geometry at hollow, bridge and top site orientations. The adsorption energy calculations show that the adsorption of pentacene molecule on Pd(100) surface is chemisorbed. For the stable adsorption geometry the electronic properties such as density of states (DOS), partial density of states (PDOS) and band structure are studied. The analysis of DOS and PDOS shows that the charge is transferred from the Pd(100) surface to pentacene molecule.

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

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From electric cars to smart phones, modern technologies require highly efficient battery power. Lithium batteries show enormous potential in this regard, but suf- fer from lack of cyclability due to dendridic electrodeposition of lithium. Dendrite formation is enhanced by certain compositions of the passivating layer formed on the anode, and supressed by others such as lithium fluoride [1]; the underlying mechanisms are not yet completely understood.

To explore these mechanisms we introduce a new, nonlinear form of polarizable continuum description for the electrolyte environment. A common failing of such polarizable continuum descriptions is that, particularly near the polar interfaces of interest to us, local microscopic electric fields are so strong that nonlinear dielectric effects must be included in the solvation framework [2]. We here show how this can be done accurately and at little additional computational cost within the framework of Joint Density Functional Theory (as implemented by [3]).

Using this new tool, we performed a first principles study of the relevant anode passivating layers. We find in particularly that the diffusion barriers for Li on LiF are smaller compared to that of LiOH and Li2O, all of which persist in the presence of different electrolytes. We propose, therefore, that the presence of LiF suppresses dendrite formation by allowing for rapid smoothing of surface inhomogeneities before dendrites can form.

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Phonon Dispersions, Electronic Structure and Photocatalytic Properties of X-doped (X=N, B and Pt) Rutile TiO_2 from Density Functional Theory

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Abstract

First principles calculations were performed on the electronic, vibrational and Raman spectra of substitutional N, B and Pt-doped rutile titanium dioxide (TiO_2), within the density functional theory (DFT), using the plane-wave pseudopotential method as implemented in the ABINIT package. Of all the photocatalytic materials TiO_2 has been shown as the most useful one, with the most efficient photoactivity, the highest stability and the lowest cost. Moreover, it is safe for humans and the environment. The development of new types of photocatalytic cells is driven by the need for clean and sustainable energy. In this respect best doped materials are considered as a promising route for departing from the traditional photocatalytic cells. The physical insight provided by computational modeling may help in developing improved photocatalytic devices. To this end it is important to obtain an accurate description of the electronic structure and phonon dynamics, including the fundamental gaps and level alignment at the doped-TiO_2 interface.

Clustering and Diffusion of Hydrogen in α-Fe Including Quantum Effects

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Irradiated materials undergo macroscopic changes which result from the interactions of defects on the atomic scale. Hydrogen contributes to embrittlement, swelling, and hardening in structural materials used in nuclear reactors, and management of these issues is crucial to the success of next-generation fission and fusion designs. The mechanisms by which these phenomena occur are not fully understood, however, vacancy-assisted mechanisms are promising. Vacancies can act as strong traps for hydrogen, which normally diffuses rapidly through bulk α-Fe. Clusters of vacancies and hydrogen atoms form bubbles, the properties of which are the subject of this density functional theory (DFT) study. We investigate the diffusion mechanisms of hydrogen and vacancies, comparing whether migration of clusters occurs through dissociation or by clusters moving as a whole. Nudged elastic band and drag methods are used to calculate environment-dependent diffusion barriers. We also describe the structure of small clusters of vacancies with varying hydrogen concentrations, finding that compact or spherical bubbles are generally lower energy than planar or linear configurations. For systems involving light elements like hydrogen, quantum effects such as zero-point energy and tunneling are very important; we include corrections for these in our calculations and discuss their importance. Calculations are performed using the DFT-SIESTA code with the Generalized Gradient Approximation (GGA).

Ab Initio Study of Magnetic Anisotropy Energy of Some Low Dimensional Systems

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We present a planewave pseudopotential density functional theory calculations of magnetic anisotropy energy (MAE) of some low dimensional systems of Fe and Co.

We show the high sensitivity of the MAE and the direction of the easy and hard axes with respect to the structure. In particular, we find that the easy axis and the MAE depend on the stacking faults and site occupancies for the Fe film on the Au(111) substrate, explaining some of the findings in the experiments. We also present our MAE calculations on the methanethiol adsorbed Co/Au(111) systems.

MAE of these quasi-two-dimensional systems being a very small quantity (~ meV), which is often close to the order of typical errors due to insufficient convergence (of parameters like k-point, planewave cutoff etc.), it needs to be calculated with an increased computational accuracy and thus is computationally more demanding .

Substarte and chemical functionalization induced magnetic moment on hexagonal boron nitride

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We have performed density functional theory calculations for studying the effect of ferromagnetic substrate (Ni(111)) and chemical functionalization (through hydrogenation) on the magnetic and electronic properties of the hexagonal boron nitride (h-BN). For the pristine h-BN sheet the top-fcc (N on top and B on fcc) and the top-hcp (N on top and B on hcp) are the two most favorable configurations with a binding energy of -0.37eV. The h-BN sheet remains insulating but becomes antiferromagnetic. Upon hydrogenating the top-fcc h-BN with 0.5 ML coverage, the H atoms can bind on two possible sites: (i) on the N atom (H-NB) and (ii) on the B atom (H-BN). Unlike the free standing semihydrogenated h-BN sheet, on the Ni surface, the H-NB configuration is energetically more stable than the H-BN configuration by 0.31eV. The 0.1 Å buckling in the pristine h-BN sheet increases to 0.45 Å for H-BN and 0.56 Å for H-NB. For H-NB, the magnetic moment of N atom is quenched completely while there is small magnetic moment of $-0.01\mu_B$ on the B atom. For H-BN, the magnetic moment contribution comes from N atom which is $-0.03\mu_B$ while the magnetic moment of B atom is quenched. The hydrogen atom in H-BN also gets a small magnetic moment of $-0.02\mu_{B.}$ On other hand the magnetic moment of the surface Ni atom is quenched significantly from $0.66\mu_B$ to $0.07\mu_{B.}$ The magnetic moments on the B or N atoms of the hydrogenated h-BN are aligned anti-parallel to the net magnetic moment of the Ni atoms. Similar results are also obtained for the top-hcp configuration.

Main Topic: A8 Catalysis and Electrochemistry

Ab initio Study of the Adsorption of NO on small Rh clusters supported on MgO

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Reduction of harmful NO gas to N_2 is an important catalytic reaction due to its practical importance in industrial pollution control processes. In this process, it is desirable to dissociate the N–O bond, for which Rh is found to be the most efficient precious metal catalyst [1]. Moreover, barriers for such dissociation processes tend to decrease on decreasing the coordination of the metal atoms [2]. Considering these two facts, adsorption and reduction of NO on both Rh surfaces [3] and their lower coordinated counterpart of small Rh clusters [4] have received particular attention in the last few years. However, in view of industrial applications, it is important to study the catalyst on some substrate support. It has been reported by our group that the NO adsorption energy increased and the effective coordination decreased on going from Rh(100) to Rh/MgO(100) [5], which might lower activation energies for NO dissociation. In spite of these studies, the catalytic activity of small Rh clusters on MgO support has not been investigated either theoretically or experimentally to the best of our knowledge. The goal of the present study is the study the catalytic dissociation of NO on MgO supported Rh clusters.

As the first step, we have studied the molecular adsorption of NO on Rh_n (n=1-4) clusters supported on MgO(100) surface using the Pwscf code of Quantum ESPRESSO. We have performed spin-polarized calculations for several different adsorption geometries. We present results on the favored adsorption geometries, binding energies and magnetic moments. We discuss the influence of the presence of the support.

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Main Topic: A3 Magnetism and Spintronics

Study of Structural, Electronic and Magnetic Properties of Pd_n, Pd_nMn_1 and Pd_nMn_2 clusters

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When small Palladium clusters are doped with Mn they undergo paramagnetic to ferromagnetic ordering giving rise to new magnetic storage materials and possessing exotic magnetic properties. We use density functional theory formalism with the spin polarized generalized gradient approximation method available in the VASP code to study the electronic, magnetic and geometrical properties of Pdn (where $n < 20$) and $PdnMn_1$, $PdnMn_2$ (where $n \leq 12$) clusters. We found that small Pd clusters exhibit magnetism in contrast to the nonmagnetic single atom Pd and bulk Pd. We also found that the icosahedral configuration is a more stable configuration as compared to the buckled bi-planer one for n=13 atom clusters for all the systems. The magnetic moments are enhanced by (3−7) μB and (2−14) μB in Pd clusters after doping with Mn and Mn_2 respectively and we also observed increased stability. Our findings also explain the origin of magnetism in the reference systems.

Application
A1 and A3

Study of Al/Al_2O_3 Interface with Reactive Force Field

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Tunneling current in aluminium oxide thin film based nano-electronic devices is strongly dependent on the geometry of a metal-oxide interface, affecting the quality of the barrier, consequently, performance of a device. Therefore, it is important to learn the structure of such interfaces and based on the knowledge of the structure understand the phenomena occurring in the devices they compound. In our study we examine three different stackings for Al/Al_2O_3 interface with the three possible terminations of the oxide, nine configurations in total. In our simulations we use reactive force-field (ReaxFF) implemented in LAMMPS molecular dynamics code. The most stable structures are identified. To validate the results density-functional theory calculations are performed additionally.

Main Topic: A5 Functional Materials

Electrocaloric effect in ferroelectric alloys from atomistic simulations

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Caloric effects, such as magnetocaloric and electrocaloric effects, have attracted a lot of attention recently in the context of increasing interest in energy conversion and renewable energy materials and devices. Here we develop and use accurate first-principles-based simulations to study electrocaloric effect (ECE) from an atomistic point of view. In particular, we develop a computational technique that allows both direct and indirect simulations of ECE within the *same* atomistic framework. We then use such a tool to provide first systematic comparison between ECE estimates obtained from direct and indirect approach which will allow us to bridge the macroscopic and atomistic description of ECE. The results of our direct atomistic simulations are then used to explore the intrinsic features of ECE in ferroelectrics with multiple transitions.

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EELS Signature of Boron Nitride Nanoribbons

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We present simulated electron energy-loss spectra for boron nitride nanoribbons using density-functional theory. The focus is specifically on the near-edge spectrum (ELNES) since this is extremely sensitive to local atomic environment and can therefore be used to detect changes in bonding around the edges or in the centre of a nanoribbon. Significant differences in the ELNES for boron atoms on the edge compared to those in the centre are predicted theoretically and confirmed experimentally. The effect of width and chirality is also investigated. Boron nitride nanoribbons have been suggested to have a range of novel properties that could be exploited in nano-electronic, optoelectronic and magnetic devices. The results presented here could be used in combination with experimental electron energy-loss spectroscopy to establish the relation between measured properties and atomistic structure.

Role of pyridine derivatives on the electronic properties of polymer/metaloxide interfaces for photovoltaics

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Hybrid solar cells formed by organic polymers and inorganic metaloxide substrates are technologically very attractive thanks to low costs, stability, and easy of synthesis [1]. Recent work on mesoporous films of titanium dioxide (TiO_2) infiltrated by poly(3-hexylthiophene) (P3HT) have shown that the use of organic interlayers formed by the small aromatic 4-mercaptopyridine molecule is able to impressively enhance the photocurrent of the solar cell [2]. In this work we adopt first-principles calculations to investigate the binding of pyridines derivatives on titania and their effect on the electronic properties. In particular, we study the energy-level alignment and the interfacial charge-transfer for different pyridine derivatives (4-mercaptopyridine, 2-mercaptopyridine, 4-tert-butylpyridine). Our results are consistent with the available experimental data and suggest new routes to improve the performances of this class of excitonic solar cells [3].

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Study of nanoconfinement of O_2 molecules in fullerenes and nanotubes

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Molecular crystalline oxygen exhibits a variety of phases as a function of an external pressure, with phase transitions accompanied by changes in the electronic and magnetic properties. An example is the so-called ε-phase, whose structure was reported by experiments performed in the last decade [1]. At 295K, under a pressure of 5.4 GPa, oxygen is solid and the phase β is accessed. Increasing pressure, at 9.6 GPa, the crystal transforms into δ phase. If more pressure is applied, around 10.0 GPa, the ε phase is observed. This phase undergoes a first-order phase transition in volume and a magnetic collapse. The oxygen molecules are displaced in a C-centered monoclinic crystal with C2/m symmetry.

With this in mind, we aim at the investigation of oxygen clusters confined in nanostructures and at the possible emergence of arrangements (at room temperature) which characterize the oxygen solid phases. Confinement is one of the most important effects in nanoscience, and it is known to affect a variety of properties of the involved molecules or particles. So, what happens with the oxygen molecules under confinement in a reduced volume? Would it be possible to access clusters with structure similar to that of the ε solid phase? In this work, we performed pseudopotential density-functional theory calculations to study the structural, energetic and also dynamical properties of nanotubes and fullerenes confining oxygen molecules. Our preliminary results show that this effect may be observed in fullerenes and carbon nanotubes, that is, the molecules tend to aggregate in O_8 clusters which, inside the nanotubes, form an oxygen nanowire. The electronic properties of the combined (nanotube + oxygen) system will also be reported.

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

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Stabilizing molecules at solid surfaces and switching them reversibly between defined states would be a key component of a future molecular nanotechnology. Adsorption at metal surfaces is of particular interest as it could lead to novel functionality in form of isomerization mechanisms not present in gas-phase or solution. Recent experiments indeed suggest such a photo-induced mechanism for tetra-tert-butyl functionalized azobenzene (TBA) at Au(111) [1], involving electron transfer from the molecule to a photo-excited hole in the metal *d*-band. Addressing this suggestion with first-principles modeling requires a numerically highly efficient approach to make the calculations of photo-excited molecular motion at the extended surface tractable. To this end we explore a density-functional theory based Delta self-consistent field approach and assess its reliability for azobenzene in the gas phase and adsorbed to Ag(111). The method predicts the overall topology of the corresponding photoisomerization pathways and the position of decay funnels fairly well. This encourages us to discuss the isomerization of azobenzene and TBA in excited states corresponding to the suggested hole-mechanism.

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Anderson localization in crystalline phase-change materials

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The study of metal-insulator transitions (MITs) in crystalline solids is a subject of utmost importance, both from the fundamental point of view and for its relevance to the transport properties of a vast class of technologically useful materials, including doped semiconductors. Very recently, a MIT was observed [1] in crystalline $\mathrm{Ge_1Sb_2Te_4}$, upon increasing the annealing temperature: remarkably, this transition was shown to be solely due to disorder. $\mathrm{Ge_1Sb_2Te_4}$ is a Chalcogenide phase-change material: this class of materials is considered to be a promising candidate for non-volatile memories of next generation [2], due to their ability to switch rapidly and reversibly between the crystalline and the amorphous phase upon heating and to the pronounced resistivity contrast between the two phases. Experimentally, $\mathrm{Ge_1Sb_2Te_4}$ undergoes a cubic to hexagonal structural transition by increasing the annealing temperature, before the MIT occurs: the cubic phase is always insulating at low temperatures, whereas the hexagonal phase displays the MIT [1]. We have carried out a comprehensive computational study of the structural and electronic properties of crystalline $\mathrm{Ge_1Sb_2Te_4}$, which has shed light on the microscopic mechanisms driving this transition [3]. For this purpose, a large number of big models (containing up to 3584 atoms) of cubic and hexagonal $\mathrm{Ge_1Sb_2Te_4}$ containing different amount of disorder in the form of a) randomly arranged vacancies and b) substitutional Ge/Sb disorder were generated and optimized using Density Functional Theory. The KKRNano [4] and CP2K [5] packages were employed for these simulations. We show that, in the cubic phase, the electronic states responsible for the transport are exponentially localized inside regions having large vacancy concentrations: this finding is corroborated by local density of states calculations and inspection of relevant wave functions near the Fermi energy. The transition to the metallic state is driven by the formation of ordered vacancy layers. Substitutional disorder and structural distortion do not play a crucial role in this MIT. The ordering of vacancies is shown to bring about a significant gain in energy and to be responsible for the structural transition as well. These results provide a step towards the goal of controlling the degree of disorder in these systems so as to tune their resistance in a reproducible fashion, which might lead to the development of devices of new concept based on multiple resistance states.

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

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Structural, elastic, electronic and optical properties of the three $CaTiO_3$ phases are studied using Density Functional Theory (DFT). Exchange–correlation effects are treated by both the Local Density Approximation (LDA) and Generalized Gradient Approximation (GGA) plus dispersion correction for the exchange and correlation potential. The equilibrium lattice constants, the bulk modulus, its pressure derivative, and the electronic structure are in good agreement with other calculations and with experimental data. The calculated band structure shows an indirect (R-Γ) band gap of 1.9 eV to cubic phase and an indirect (Γ-X) band gap of 2.31 eV to tetragonal phase. To the orthorhombic phase the band gap was direct (Γ- Γ) of 2.41 eV, all the results obtained with the GGA approximation. The calculated DOS are in reasonable agreement with the experimental energy spectra and the features in the spectra are interpreted by a comparison of the spectra with the PDOS. From the DOS analysis, as well as charge-density studies, we conclude that the bonding between Ca and TiO_3 is mainly ionic and that the TiO_3 entities bond covalently. The calculations of the effective mass of the electron and hole carriers were also conducted, to our knowledge, no data are available in literature for comparison. The real and imaginary parts of the dielectric function and hence the optical constants such as refractive index and extinction coefficient are calculated. The calculated spectra are compared with the experimental results for $CaTiO_3$ and are found to be in good agreement with the experimental results.

Theory and Methods:
T1 Density-Functional Theory beyond LDA

Applications:
A11 Other applications

A comparative study of density functional methods for the optical properties of TiO_2 nanowires

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Available linear response time dependent density functional theory calculations failed to properly describe optical properties of low dimensional TiO_2 structures. We attempted to get reasonable absorption spectra for anatase TiO_2 nanowires having (101) and (001) facets from first principles computations. We performed pure, hybrid and beyond DFT calculations including supplementary Hubbard U on-site repulsion, range separated screened Coulomb exchange and GW quasiparticle corrections. The results obtained by these methods have been compared. We investigate the effect of size and geometry on the optical spectra of TiO_2 nanowires. Absorbances of anatase nanowires have also been discussed in relation to those of the bulk, surface and finite titania structures.

First-principles study of the structural and dynamical properties of $SrRuO_3$

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$SrRuO_3$(SRO), as a popular electrode material, has fascinated researchers for many years due to its surprising itinerant ferromagnetism, unusual transport properties, and the degree and consequences of correlation. Here, by means of first-principles calculations, we investigate the structural and dynamical properties of $SrRuO_3$(SRO) with different approaches (PW-LDA, WC-GGA and hybrid B1-WC functionals). The full phonon dispersion curves of the high-temperature cubic phase of SRO are reported and compared to available experimental data. We find a branch of unstable antiferrodistortive (AFD) phonon modes extending from *R* to *M* points of Brillouin zone. We describe how cubic SRO can be turned to its *Pnma* ground state by introducing different rotations of oxygen octahedra associated to unstable AFD modes. The zone-center phonon modes of this *Pnma* ground state are also reported. The energetics of different intermediate phases are computed and will be used for building an effective hamiltonion giving access to the finite temperature properties and structural phase transitions of SRO.

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

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The adsorption of hydrocarbon molecules on carbonate and silicate surfaces was studied by means of first-principles calculations. The calculations were based on the Density Functional Theory (DFT) with solid state Nuclear Magnetic Resonance (NMR) and simulation of noncontact Atomic Force Microscopy (nc-AFM). Energetic, electronic, structural and kinetic properties have been determined for the adsorption of the representative hydrocarbons (benzene, toluene and hexane) on carbonate (calcite ($CaCO_3$) and quartz silica (SiO_2)) surfaces. Our results suggest that Ca sites are the most energetically favorable for hydrocarbon adsorption on carbonate systems. The calculations also indicate a weak interaction between the hydrocarbon molecules with the bare silica surface for all hydrocarbons studied. In this context, the Gauge-Including Projector Augmented Wave (GIPAW) method was used to compute solid-state NMR parameters for ^{43}Ca in calcite surfaces and ^{29}Si in silica surfaces using periodic boundary conditions through the QuantumEspresso code. It was possible to assign the peaks in the NMR spectra for all structures studied and determine the force distance models based on simulated AFM. A chemical shift differentiation for atoms located on different sites (bulk and surface) was observed for both calcite and silica systems. The presence of hydrocarbon molecules also modifies the chemical shift of adsorbed Ca and Si sites with respect to the pristine and isolated surfaces. Even though the interaction of the benzene molecule with the calcite/silica surfaces is weak, there is a very sizeable displacement of the signal of the Ca and Si atoms over which the hydrocarbon molecule is located. A similar effect has been also observed for hexane adsorption in both surfaces.

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

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Direct Alcohol Fuel Cells (DAFC) are interesting electrochemical devices due to their high energy density, low pollutant emission, no need of an external reformer and low operating temperature. Ethanol is an ideal choice as fuel for DAFCs because of its high mass energy density, nontoxicity, and its availability from renewable biomass sources. The ethanol efficiency as a fuel in DAFC is closely related to the selectivity of the catalyst toward CO_2 production. Even for the most effective catalysts the total oxidation is not observed and the development of catalysts for efficient ethanol oxidation is required [1,2]. We apply first principles calculations to explore the ethanol electrochemical oxidation over Pt(111) and Pt/Pd(111) surfaces. The structural and energetic properties of the intermediates products in the acetic acid and CO pathways were investigated with the inclusion of van der Waals interactions. Dispersion-corrected Density Functional Theory calculations (DFT-D3) [3] were carried out using the Vienna Ab initio Simulation Package (VASP). The exchange and correlation terms were treated in the Generalized Gradient Approximation (GGA) of Perdew-Burke-Ernzerhof (PBE), and projector-augmented potentials were used. Our results suggest that acetic acid pathway is more favorable. Even more, our DFT-D3 calculations show that in the end of the reaction pathway acetic acid desorbs from the surface. These results are in agreement with experimental observations since during electrochemical oxidation of ethanol over Pt-based catalysts acetic acid is one of the most abundant products. The structures within reaction pathways were explored through First Principles simulation of noncontact Atomic Force Microscopy (nc-AFM). From the simulated images, it is possible to characterize the ethanol reaction steps to acetic acid and CO production. The calculations show that for all intermediate species the C-C bond are practically parallel to the surface. This trend was not observed within standard DFT calculations. The transitional states were determined, and atomic hydrogen is adsorbed at the fcc and top site of the surface, in agreement with our previous results for H adsorption at metallic layered supported nanofilms [4]. Calculated AFM forces allow the differentiation between the different chemical sites. H and O sites are very similar for CH_3CH_2OH, CH_3CO, CH_2+CO and CH_2COOH. For C sites the differences are more pronounced and can be used to characterize the different chemical environment.

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

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Chlorogenic acids are a family of esters formed between certain trans-cinnamic acids and quinic acid (1L-1 (OH),3,4/5-tetrahydroxycyclohexane carboxylic acid), which has axial hydroxyls on carbons 1 and 3 and equatorial hydroxyls on carbons 4 and 5. Results of infrared absorption and Raman spectroscopy in combination with a systematic quantum mechanical study is reported for the chlorogenic acid isomer 3-CQA (1R,3R,4S,5R)-3-{[(2E)-3-(3,4-Dihydroxyphenyl)prop-2-enoyl]oxy}-1,4,5-trihydroxycyclohexanecarboxylic acid), a major phenolic compound in coffee. The equilibrium geometry, harmonic vibrational frequencies, infrared intensities and activities of Raman scattering were calculated by density functional theory (DFT) employing B3LYP functionals using the 6-311G(d,p) basis set with complete relaxation in the potential energy surface. The calculated wavenumbers after proper scaling show a very good agreement with the observed experimental values. The electrostatic potential mapped onto an isodensity surface has been obtained. A natural bond orbital analysis (NBO) has been performed in order to study intramolecular bonding, interactions among bonds, and delocalization of unpaired electrons. HOMO-LUMO studies give insights into the interaction of the molecule with other species. The calculated HOMO and LUMO energies indicate that a charge transfer occurs within the molecule.

Main Topic: A1 Nanoscience

Topological defect formation and activation in carbon nanostructures

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Topological defects such as Stone-Wales defects play a crucial role in growth, fusion, mechanical and catalytic properties of carbon nanostructures. For both fullerene and carbon nanotube, our first-principles calculation shows that single substitutional doping reduces the Stone-Wales activation barrier substantially due to local bond distortion and softening. In addition, for CNTs both formation and activation energies of these 5-7-5-7 defects strongly depend on the chiral vector (and thus on the nanotube radius), and the orientation of the defect. We rationalize our results via studying the bonding charge density and phonon spectra.

Microscopic charge fluctuations in hexagonal boron nitride

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We present an *ab initio* approach to the electron dynamics through the calculation of the total polarizability matrix, including the off-diagonal elements. The charge density induced in a system by an external perturbation is computed in real space and time, following the idea of Abbamonte *et al.* [1]. The difference between our approach and the one from Ref. [1] is that we can calculate not only the diagonal response $\chi(\mathbf{q},\mathbf{q},\omega)$, but also the off-diagonal elements of the matrix $\chi(\mathbf{q},\mathbf{q}',\omega)$. Hence, we have access to the microscopic charge oscillations which are induced by the local-field effects.

We have studied these charge oscillations at various frequencies comprising interband-transition and plasmon-excitation energies. The real-space approach allows us to see which electrons (or orbitals) contribute to which kind of excitation. The final goal is to offer theoretical support and benchmark to future inelastic x-ray scattering experiments that may measure also the off-diagonal elements of the polarizability.

The method is applied to hexagonal boron nitride (h-BN) which is the most stable of the three existing structures (hexagonal, cubic, and wurtzite) at room temperature and ambient pressure. Because of its thermal stability it is a widely used material in vacuum technology. The interest in h-BN has been renewed by the possibility of preparing boron-nitride nanotubes that are far more resistant to oxidation than carbon nanotubes and, therefore, suitable for high-temperature applications [2].

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Ideal Energy-Level Alignment at the ZnO/P3HT Photovoltaic Interface

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Hybrid organic-inorganic photovoltaic devices comprising P3HT and ZnO have attracted considerable interest due to the possibility of solution processing and the favorable interfacial energy-level alignment. Despite the tremendous progress that has been made in enhancing power conversion efficiencies, however, these devices still suffer from low short-circuit currents and moderate open-circuit voltages. A detailed examination of the atomic-scale physics underlying the energy-level alignment at the ZnO/P3HT interface is therefore critical if we are to understand what is the maximum ideal open-circuit voltage for this class of solar cell. Here we present the results of a first-principles study [1] on large model interfaces between ZnO and P3HT. Using a combination of density-functional theory (DFT) and post-DFT methods based on hybrid functionals, we examine the structure and energetics of the semiconductor/polymer interface, as well as the interfacial energy-level alignment. We analyze the effect of charge transfer on the ideal open-circuit voltage and identify a failure in the standard electron affinity rule. We determine a maximum ideal open-circuit voltage of ∼2 V, which suggests that there is significant room for enhancing the performance of ZnO/P3HT solar cells by optimizing the interface at the nanoscale.

Acknowledgements

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Main Topic: A10 Materials Design

FIRST-PRINCIPLES CALCULATIONS OF THE STRUCTURAL AND ELECTRONIC PROPERTIES OF ZINC BLENDE $B_xIn_{1-x}N$

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We present first-principles calculations of the Structural and electronic properties of zinc blende for different concentrations x of ternary alloy $B_xIn_{1-x}N$. The computational method is based on the pseudopotential method as implemented in the Abinit code. The exchange and correlation energy is described in the local density approximation (LDA), generalized gradient approximation (GGA) and also the quasiparticle approximation(GW). We have investigated the effect of composition on the lattice parameters, bulk modulus and band gap of the zinc blende BN, InN. The results obtained are in a good agreement with experimental and theoretical values concerning the variation of the gaps and crossover from direct to indirect band gap and the bowing parameter.

The effect of ligand adsorption on the structure of metal nanoparticles

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Metal nanoparticles are perhaps one of the most outstanding applications of nanotechnology due to the imminent use of these nanostructures on diverse fields, i.e. biosensors, catalysis, drug "delivery" and construction of nano-circuits.

Colloidally prepared metal nanoparticles are gaining attention for catalytic applications because of the advanced possibilities to tailor their size and shape, which are often important factors governing catalytic activity and selectivity. In the case of bimetallic catalysts, composition is usually difficult to control by traditional techniques, but by colloidal chemistry the relative portions of the metals in the nanoparticles can be exactly predefined. This approach offers the advantage of controlling structure and composition of the resulting particles.

Preparation, conservation and protection of metallic or multimetallic nanoparticles usually require protection with organic ligand molecules if they will remain in a colloidal suspension. When nanoparticles are made of gold, a relatively easy way of protect them is through molecular self-assembly, particularly with thiols molecules due to the strong interaction between sulfur and gold atoms. Self-assembled monolayers (SAMs) have been intensively studied, at experimental[1, 2] and theoretical level, on extended gold (111) surfaces[3, 4] and small Au clusters[5, 6, 7].

In the present work we show the application of a new semiempirical potential, recently developed in our Lab, to describe molecule-metal interfaces in a more realistic way[8]. This potential uses Density Functional (DFT) calculations in combination with the bond-order concept, and is simple and easy to implement in standard MD/MC codes. In particular we show the effect of soft and hard surfactant on the structure of gold and palladium nanoparticles larger than 1nm.

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Scattering potentials of defects on Ge(001) surfaces

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As new techniques for the nanoscale manipulation and modification of materials progress, the electron scattering properties of nanostructures are the focus of attention both experimentally and theoretically. Although scanning tunneling microscopy and mechanically controllable break junctions have been used to examine the scattering properties of nanoscale systems sandwiched between two electrodes, it is not easy to discuss the contribution of local chemical bonds to the electron scattering using these techniques. On the other hand, the spatial maps of the local density of states obtained by scanning tunneling spectroscopy can give us the images of standing waves, which provide important information about the dispersion relation of the electron scattering process at the potential barrier.

In the first-principles calculations based on the density functional theory for examining the transport properties of nanostructures, the scatterers are suspended between two electrodes that extended semi-infinitely and are connected to bulks; thus, electron wave functions extending over the entire system can be correctly described as a scattering state distributed as a result of the existence of defects when an electron comes from infinitely deep inside the electrode. However, few studies have attempted to obtain an understanding of the relationship between the scattering potential and the spatial maps of the local density of states.

I examined the scattering potential of the defects on Ge(001) surfaces using a first-principles calculation[1]. By calculating the scattering wave functions using the overbridging boundary-matching method[2], the standing waves in the spatial map of the local density of states are examined; the waves correspond to the image of the differential conductance obtained by scanning tunneling spectroscopy[3]. The period of the standing wave and its phase shift agree with those obtained by the experiment. I found that the scattering potential acts as a barrier when the electronegativity of the upper atom of the dimer is larger than that of the lower atom, while it becomes a well in the opposite case. The scattering potential is related to the stabilization of the π bands of the Ge(001) surface due to the difference in electronegativity between Ge and the impurity.

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Main Topic: A 7 Spectroscopies

Optical properties of ordered defect compounds for $CuIn_5Se_8$ and $CuIn_3Se_5$: An ab-initio study

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Full potential linear augmented plane wave method is used to perform electronic and optical properties of ordered defect compound (ODC) $CuIn_5Se_8$ and $CuIn_3Se_5$. The supercells are generated with parent chalcopyrite structure of $CuInSe_2$. The band structure and density of state of ODC's are discussed in terms of parent chalcopyrite compound $CuInSe_2$. The dielectric function real $\varepsilon_1(\omega)$ and imaginary $\varepsilon_2(\omega)$ part of $\varepsilon(\omega)$ as well as the complex refractive index and normal-incidence reflectivity are calculated. The optical absorption peaks in the $\varepsilon_2(\omega)$ are explained in the terms of band structure and density of states. The upper valence bands of ODC's are exclusively formed by the p-d hybridization of Cu-3d and Se-4p states. The obtained results are in good agreement with the experimental data over the entire range of photon energies. The calculated threshold values for $CuInSe_2$ and ODC's are underestimated. The chemical trends are also discussed.

Calculating quasiparticle energy-level alignments at molecule/semiconductor interfaces

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Molecules adsorbed on semiconductor surfaces are ubiquitous in nanotechnology research. In dye-sensitized solar cells, where photocurrent generation relies on the type-II alignment of the discrete molecular energy levels with the bands of the semiconductor, developing a quantitative understanding of the electron energetics at the molecule/semiconductor interface is an essential step towards rational strategies of device optimisation. Here, we develop a procedure for calculating quasiparticle energy-level alignments from first principles at complex molecule/semiconductor interfaces [1]. We illustrate our method by considering the prototype dye-sensitized solar cell interface of the N3 molecule adsorbed on the anatase TiO_2 (101) surface [2]. Our work combines DFT calculations on large interface models, $GW + U$ calculations on bulk TiO_2 [3] and ΔSCF calculations on the N3 molecule adsorbed on a TiO_2 nanoparticle. The latter allows a direct evaluation of the substrate-induced renormalization of the molecular energy levels, which occurs through both classical image-charge screening and direct charge transfer. We consider broadening due to configurational disorder and temperature through Car-Parrinello MD simulations of large interface models. The energy-level alignment calculated including quasiparticle and image-charge corrections is in quantitative agreement with that measured in photoemission experiments, illustrating the vital role played by many-body effects at these interfaces.

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Fundamental limits on transparency: first-principles calculations of absorption

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Transparent conducting oxides (TCOs) are a technologically important class of materials with applications ranging from solar cells, displays, smart windows, and touch screens to light-emitting diodes. TCOs combine high conductivity, provided by a high concentration of electrons in the conduction band, with transparency in the visible region of the spectrum. The requirement of transparency is usually tied to the band gap being sufficiently large to prevent absorption of visible photons. This is a necessary but not sufficient condition: indeed, the high concentration of free carriers can also lead to additional optical processes: direct absorption to higher conduction-band states or indirect absorption mediated by phonons or defects. A fundamental understanding of the factors that limit transparency in TCOs is essential for further progress in materials and applications.
Our calculations are the first to address indirect free-carrier absorption in a TCO completely from first principles. We present results for SnO_2 [1], but the methodology is general and is also being applied to ZnO and In_2O_3. The calculations provide not just quantitative results but also deeper insights in the mechanisms that govern absorption processes in different wavelength regimes, which is essential for engineering improved materials to be used in more efficient devices. For SnO_2, we find that absorption is modest in the visible, and much stronger in the ultraviolet and infrared.
This work was supported by DOE, NSF, and BAEF.

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Atomic-scale insight into self-segregation and diffusion processes on a Ni/Cu bimetallic surface

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Achieving control of the nano-scale structure of binary alloys is of paramount importance for the design of novel materials with specific properties, leading to e.g. improved reaction rates and selectivity in catalysis and controlled growth of nanostructured materials like graphene. A peculiar example is the NiCu bimetallic alloy and in particular its surface. Ab-initio Density Functional calculations in the spin-polarized Generalized Gradient Approximation, combined with in-situ real-time spectroscopy [1], show that the complex self-diffusion mechanisms determining the key properties of the NiCu can be mostly defined by kinetic rather than energetic effects. We show that Ni-Ni interaction plays an important role in the Ni-Cu exchange process, which is at the basis of Ni migration into the bulk and segregation to the surface. We also show that the Ni segregation barriers are strongly influenced by the local Ni concentration, suggesting that nano-scale control of self-diffusion and segregation processes close to the surface can be achieved by finely tuning the relative concentration of the alloy constituents.

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Applications:
A6 Surfaces
A10 Materials Design
A1 Nanoscience

First principle study of donor wave functions in silicon nanowires

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The localization of the donor electron wave function can be of key importance in various silicon application, since it determines the interactions between neighbouring donors and influences the charge density close to the donor atom. These properties are important in light of applications like nuclear spin qubits [1] based on the hyperfine interaction between electron and nuclear spin [2] or for determining the critical density of metal-insulator transitions [3]. In particular the delocalization is a critical feature when dealing with nanostructures, where the confinement induces a squeezing of the donor wave function.
Using fully ab-initio calculations, we have studied the delocalization of the donor electron wave function along the axis of a nanowire with different orientations and for phosphorus and selenium donors. We show that the shape and delocalization is greatly influenced by the orientation of the nanowire and that a considerably larger value can be obtained for [011] oriented nanowires, compared to [001] and [111] orientations. We also demonstrate that its value can be controlled by applying a compressive or tensile uniaxial strain. As a last result we show the effect of the delocalization on the hyperfine parameters, that can be calculated with projector augmented-wave method (PAW) [4].

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Main Topic: A10 Materials Design

The evaluation of perovskite phase transitions using AIDA, a materials informatics platform for materials design and discovery

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First-principles high-throughput screening of novel materials is emerging as a new frontier in materials design. A key challenge is the need to establish a "materials' informatics" infrastructure able to automatically prepare and execute calculations for large classes of materials, monitor calculations, and store, retrieve and analyze complex data. To this aim, we are developing a powerful and flexible platform named AIDA ("Automated Infrastructure and Database for Ab-initio design") that allows to automatically submit calculations to a cluster, retrieve results when the jobs finish, parse the results and store them in a database. Thanks to this tool, a researcher becomes unencumbered by the most tedious tasks of a calculation, more complex properties become routinely available, and permanent tracking and storage of all the calculations steps becomes straightforward.
As a first application, we show some results on the phase stability of perovskite materials, and in particular the evaluation of the phase-transition critical temperatures for the cubic, tetragonal, orthorhombic, and rhombohedral phases of some of these systems. Moreover, we perform a systematic study on the unpolarized cubic phase of a representative family of perovskites. Our results indicate that there is no unique model that can explain this phase; on the contrary, while some systems are consistent with a displacive or an order/disorder model, others can sustain a stable displacement pattern of B-site cations in a $2 \times 2 \times 2$ supercell, while still having a zero net polarization.

First-Principles Study on Carbon Emission Process at 4H-SiC(0001) Surfaces and 4H-SiC(0001)/SiO_2 Interfaces

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SiC is attracted much attention due to its high breakdown strength. However, the SiC/SiO_2 interface is suffered from a large amount of interface defects which is generated during the oxidation of the SiC substrate. The result of secondary ion-microprobe mass spectrometer experiment shows that the most of C atoms do not remain at the interface after the thermal oxidation since the C signal near the interface is under the detection limit [1]. On the other hand, high-resolution transmission electron microscopy observation indicates that the SiC/SiO_2 interface is not structurally and chemically abrupt [2]. A controversial topic regarding the SiC/SiO_2 interface is the interfacial atomic structure during the oxidation process of SiC. In this study, we investigate the C emission process from the 4H-SiC(0001) surface and 4H-SiC(0001)/SiO_2 interface using first-principles calculations.

We calculate the energies of the CO emission by sequentially inserting O atoms between Si-C bonds around a particular C atom at the 4H-SiC(0001) surface and 4H-SiC(0001)/SiO_2 interface, and removing the C atom as a form of CO. For the SiC/SiO_2 interface model, the SiO_2 on the SiC surface is chosen as β-tridymite SiO_2 (001) since the interface has the small lattice mismatch of ~1.5%. The formation energy is calculated by $E_{\mathrm{w/o}}$-[$E_{\mathrm{w/}}$+μ_{CO}], where $E_{\mathrm{w/o}}$ and $E_{\mathrm{w/}}$ are the total energies without and with the CO emission, respectively, and μ_{CO} is the chemical potential of the CO molecule. Figure 1 shows the energies of the CO emission at the surface and interface with respect to the number of the O atoms inserted. When the number of the O atoms inserted is three, the CO emission is preferable both at the surface and interface since the perfect SiO_2 network remains after the CO emission. The energy gain of the CO emission from the interface is greater than that from the surface because the interface stress is relaxed by removing the CO molecule from the SiC/SiO_2 interface. In the presentation, we also discuss the CO emission from the SiO_2 bulk.

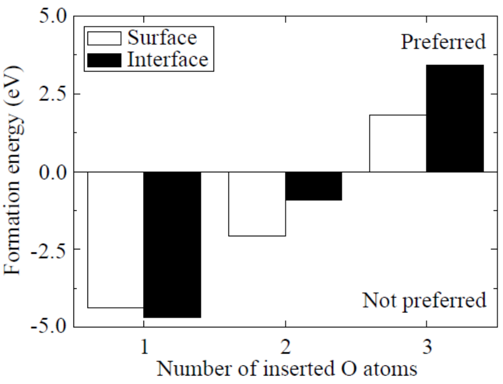

FIG. 1. Formation energy of CO emission at surface (white bars) and interface (black bars) with respect to number of O atoms inserted.

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Influence of Al concentration on the opto-electronic properties of Al-doped MgO

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We use density functional theory (DFT) within the local-density approximation (LDA) to investigate the structural, electronic, and optical properties of Al-doped MgO. The concentrations considered range from 6% to 56%. In the latter case, we also compare the optical properties of the pseudo-amorphous and crystalline phases. We find that, overall, the electronic properties of the crystalline phases change qualitatively little with Al concentration. On the other hand, the changes in the electronic structure in the pseudo-amorphous phase are more important, most notably because of deep impurity levels in the band gap that are absent in the crystalline phase. This leads to observable effects in, e.g., the optical absorption edge and in the refractive index. Thus, the latter can be used to characterize the crystalline to pseudo-amorphous transition with Al doping level.

DFT Studies on the Adsorption of Atomic Sulfur and Methanethiolate at Coinage Metal Surfaces

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Density-functional theory (DFT) calculations have been employed to study the adsorption of atomic sulfur and methanethiolate at Cu(111), Ag(111) and Au(111) surfaces. A large number of surface models has been investigated considering a variety of adsorbate phases, binding sites, and surface coverages at the ideal as well as the reconstructed surface. The results show that the adsorption of atomic sulfur and methanethiolate gives rise to several surface reconstructions. The most stable phase for atomic sulfur at Cu(111) and Ag(111) is a $(\sqrt{7}\times\sqrt{7})R19.1^\circ$ reconstruction containing three sulfur atoms in the unit cell and three metal adatoms in the reconstructed layer. For methanethiolate, the most stable phases are different for each metal. The proposed $\begin{bmatrix} 5 & 0 \\ 1 & 3 \end{bmatrix}$ supercell generally used to approximate the experimentally observed pseudo-(100) phase at Cu(111) yields the lowest surface energy. However, the calculated structure deviates from the perfect fourfold Cu-S coordination observed in STM. The $(\sqrt{7}\times\sqrt{7})R19.1^\circ$ reconstruction is found to be the most favored phase for methanethiolate at Ag(111). In contrast to atomic sulfur, the unit cell contains five silver atoms in the reconstructed layer, resulting in an approximately fivefold Ag-S coordination. For Au(111), we find that the most preferable adsorbate phase contains complexes of an Au adatom bound to two thiolate radicals. A very similar surface energy was obtained for the adsorption of this complex in three Au(111) supercells: a cis-form in a c(4×2) cell, a trans-form in a (3×4) cell and a trans-form in a $(3\times4\sqrt{3})$ cell. All cases have the same coverage of 1/3 monolayers and an adatom/thiolate ratio of 1/2.

CHP molecule filling the pores of the *h*-BN/Rh(111) nanomesh: A computational study

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In nanotechnology there is a quest for finding an efficient and precise way of placing the components elements in the system. A bottom-up approach to achieve this is to use templating, targeting for example the molecular constituents to attach at the appropriate site. One way to reach such a guiding is the modulation of the potential energy landscape for molecules landing on a surface.

One such system is the *h*-BN/Rh(111) *nanomesh*, that consist of a commensurate unit cell of 3.22 nm [1]. This structure exposes both *pores*, areas with close contact to the substrate, and *wires* that is farther away from the metal surface. The different areas lead to a laterally varying of the local work function [2].

We have performed density functional theory calculations on the adsorption of hexa-iodo-cyclohexa-m-phenylene molecule (CHP) on the nanomesh. The supercell is laterally 13×13 units of *h*-BN on 12×12 cells of Rh(111) surface. Because the interactions both between the *h*-BN overlayer of the nanomesh and the substrate metal and the molecule with the nanomesh are weak, we include an empirical van der Waals interaction between the atoms. We investigate both the adsorption mechanism of the CHP molecule in the pore of the nanomesh as well as the dissociation of the molecule by the extraction of the iodine atoms from the organic body of the molecule. These results agree well with the scanning tunnelling microscopy at EMPA, Switzerland.

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Electronic structure calculations on MX_2 dichalcogenide/Graphene hybrid structures.

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Since the first isolation of graphene in 2004 [1] there has been much effort in exploiting its outstanding electronic properties [2] to technological applications, in particular, in combination with other two-dimensional crystals. Nowadays, transition metal dichalcogenides such as MoS_2 and WS_2 are bringing much attention due to the fact that, although in nature they exhibit a bulk structure, they are layered materials which can be exfoliated like graphene to produce 2D single or multi-layer structures [3]. Interestingly, they are semi-conductors with a change in their electronic structure properties when changing from bulk (which presents an indirect gap) to a single layer (with a direct gap). This opens up new possibilities for the creation of new electronic and optoelectronic devices.

Here, we present *ab initio* DFT calculations (done using the SIESTA code [4]) of the electronic properties of single-, multi-layer and bulk MoS_2 and WS_2. We find parameters for a Tight Binding model that describes these systems. Finally, we study the interaction of these materials with graphene and the possibility of fabricating new devices with these hybrid structures [5, 6].

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Structural and Electronic Properties of IV Nanowires: Ab-initio Study

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Ab-initio self-consistent study has been performed to analyze the stability of IVth group elemental linear nanowires such as silicon (Si), germanium (Ge) and lead (Pb) in their linear atomic configuration. Using the revised Perdew- Burke- Ernzerhof (revPBE) parameterization of generalized gradient approximation (GGA) potential the geometries have been optimized. Pb nanowire possess the lowest total energy and can be stated as the most stable linear structure amongst the other two The ground state parameters such as bulk modulus, first order pressure derivative and equilibrium lattice parameters for different linear nanowires have been computed. The calculated bulk moduli are decreasing from Si to Pb, suggesting that Si linear nanowire is mechanically much stronger than rest too. The variation of lattice parameter and bulk modulus with respect to different structures has been shown in figure. The electronic band structures, density of states for different linear nanowires have also been analysed, where the metallic behavior has been observed in all the nanowires, in contrast to the semiconducting nature of bulk Si and Ge.

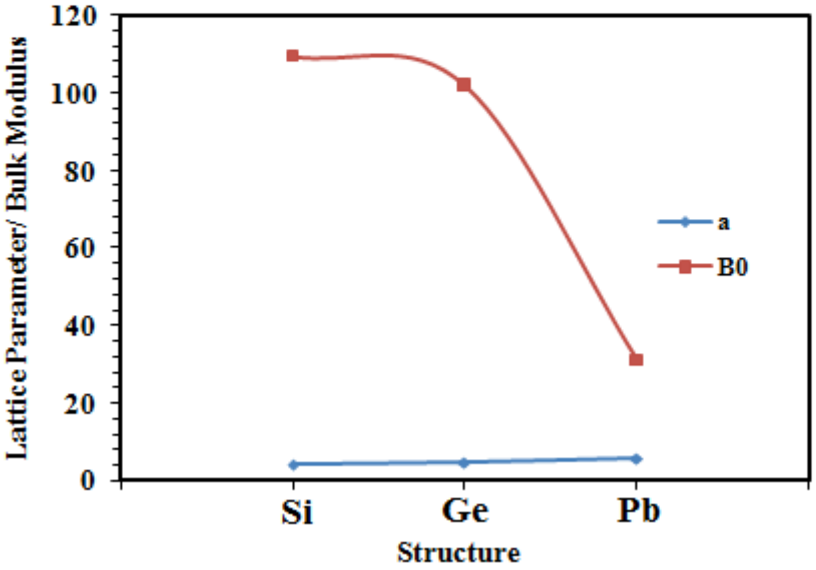

Figure- Variation of Lattice parameter (a) and bulk modulus (B_0) with different structures.

Size dependent electronic properties of ZnO nanowire: Ab-initio study

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ABSTRACT

First principle density function theory based approach has been used to analyze the structural stability and electronic properties of ZnO nanowire in the zincblende (B3) type phase. The structural stability of the material has been analyzed in terms of total energy as well as binding energy computed using local density approximation (LDA) with the Perdew-Zunger (PZ) parameterization. The study finds that the B3 type phase of ZnO nanowire is stable at different diameters and in comparison to its semiconducting bulk counterpart, the linear nanowire of ZnO same is metallic in all the three diameters 0.4nm, 0.6nm and 0.8nm, taken into consideration. Study also computes the ground state properties of these different sized nanowires.

Keywords: ZnO, Nanowire, First principle, Zincblende

Optimal interface doping at $\mathbf{La_{2/3}Sr_{1/3}MnO_3/SrTiO_3(001)}$ heterojunctions for spintronic applications

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Due to its large spin polarization and high Curie temperature, $La_{2/3}Sr_{1/3}MnO_3$ (LSMO) is a promising candidate for spintronic applications, such as tunneling magnetoresistance and field-effect transistors. With $SrTiO_3$ (STO) as insulating barrier, the resulting LSMO/STO/LSMO(001) magnetic tunneling junctions were found to give rise experimentally to an exceptionally large tunneling magnetoresistance (TMR) ratio at low temperatures. However, the TMR was found to depend strongly on interface effects and to vanish well below the LSMO Curie temperature. Previously, it was also observed experimentally that doping the SrO-terminated STO-LSMO, by depositing two unit layers of $LaMnO_3$ at the interface, strengthens the interface ferromagnetism and enhances the TMR ratio. Nonetheless, the effect was not large enough to make the SrO-termination competitive with the TiO_2 termination.

We apply the first-principles density-functional-theory method to explore the effects of doping at the LSMO/STO(001) TiO_2-terminated interface. Both the generalized-gradient approximation (GGA) and the GGA plus on-site Coulomb interaction approach (GGA+U) are used. In our simulations, one unit layer of LSMO at the interface is replaced by $La_{1-x}Sr_xMnO_3$, with varying doping $0 < x < 1$. In particular, we are interested in the variations of the exchange energy, $E_{AFM} - E_{FM}$ (energy difference between antiferromagnetic and ferromagnetic alignment of the MnO_2-interface layer relative to bulk LSMO), as a measure of the robustness of the interface ferromagnetism for spintronic applications. The corresponding optimal doping is found to be very close to $x = 1/3$, both in GGA and GGA+U. This is also the composition which gives the maximum $p-$type Schottky barrier height in our calculations.

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

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Epitaxial graphene on metals, in analogy to ultra-thin films of alkali-halides and oxides,[1,2] can be used to decouple the electronic states of molecular adsorbates from the substrate, and allow the visualization of their orbitals with intramolecular resolution.[3,4] In the case of a strong interaction with the underlying metal, however, the electronic structure of graphene is strongly perturbed,[5] and such modification can have unexpected consequences on the properties of the molecular overlayer. As a prototypical example of this situation, we have studied the adsorption of the electron acceptor 7,7',8,8'-tetracyanoquinodimethane (TCNQ) on monolayer graphene grown on Ru(0001). Using large-scale calculations based on Density Functional Theory (DFT),[6,7] we have characterized the role of charge-transfer at the interface, as well as the nature of the lateral interactions that are at the origin of the formation of highly ordered molecular monolayers.

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

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Silicon Carbide (SiC) has unique properties making it suitable for hard and protective coatings, optoelectronics and sensing. It is the most promising alternative to Si for electronics devices working at high power/high frequency or in prohibitive conditions. A new perspective is now being pursued for SiC as material for biomedical applications. Being the substrate for synthesizing high quality Graphene, SiC is expected to be one the most promising interface for Graphene-based electronics.

Despite the use of different growth approaches, SiC synthesis of high quality/low defects crystalline films still represents an open challenge. In particular, SiC heteroepitaxy on Si is interesting for the cubic (3C) polytype synthesis, having potentially the best electrical properties. In this case, Molecular Beam Epitaxy (MBE) has demonstrated to be a viable approach to 3C-SiC/Si synthesis at ~1200 K, using buckminsterfullerene (C_{60}) as C precursor. The epitaxy is critically affected by three factors: high lattice/thermal mismatches between SiC and Si, the material processing temperature (T), typically higher than 1100 K, and Si diffusion through the SiC film, creating defects at the nano and micro-scale. Therefore, synthesizing SiC at lower T is highly desirable to reduce side-growth processes, film defectivity and production costs.

In this work we demonstrate the room T (RT, 300 K) synthesis of nanocrystalline 3C-SiC on the Si(111)7×7 surface based on the Supersonic Molecular Beam Epitaxy (SuMBE) approach, where C_{60} translational kinetic energy (KE) reaches values of 30-35 eV undergoing an aerodynamic acceleration in vacuum. Chemical process are activated on the Si surface by the high KE of the C precursor. Furthermore, we simulate the C_{60}-Si(111)7×7 collision by Density Functional Theory (DFT) and we show that, to obtain the cage rupture at the observed kinetic energies, one needs to go beyond the Born-Oppenheimer (BO) approximation and use non-adiabatic molecular dynamics (NA-MD) to intertwine the electronic and nuclear motion.

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Main Topic: A1 Nanoscience

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

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Since their discovery of fullerenes(1) and carbon nanotubes(2) have received tremendous both experimental and theoretical research on the related materials. In 1998(3), while Luzzi and his group were studying purified open-ended single-walled nanotubes they found accidentally that fullerenes were incorporated inside nanotubes, like many peas in pod(4) so called 'nanopeapods'. This hybrid nanocarbon materials have unique structures and extraordinary properties in fact this materials can be thought as a functionalized nanotube where the electronic structure of the host speices is modified and controlled by the encapsulated species(5). So they are important for technological applications such as recording devices and quantum computations.

In this study we take (8,8), (9,9) and (10,10) carbon nanotubes like host species. For one-dimensional chains of C60 like encapsulated sipecies, we take different positions that hekzagon-hekzagon, hekzagon-hekzagon edge, pentagon-pentagon and pentagon-pentagon edge. The results indicate that the electronic features changes interestingly for these 12 positions.

Our total –energy calculations are carried out within the local density approximation (LDA) in the density functional theory (DFT). We use a plane wave basis set with a cut off energy of 200 Ry to expand the valence wave functions. To describe the electron-ion interaction used norm-conserving *ab-initio* pseudopotentials generated by using the Troullier-Martins scheme. In our calculations the geometry is optimized within the conjugate gradient approach and fort he full Brillouin zone used two k-points.

In summary, optimized geometries for various orientation of a chain of C60 molecules encapsulatd in different carbon nanotubes have been calculated. It is shown that from the bands structures above, the electronic structure of the (10,10) and (9,9) peapods is not a simple sum of fullerenes and nanotubes. However the rotation of the incorporated C60 molecules can effect the electronic properties of the peapods because the orbital hybridization between fullerenes and SWNTs depends on the orientation of the former insde the latter; so th overlapping integrals.

Theory and Methods:
T1 Density-Functional Theory beyond LDA

Applications:
A1 Nanoscience
A5 Functional Materials

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

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Binary bismuth chalcogenides Bi_2Se_3, Bi_2Te_3, and derived materials are currently justified as the reference topological insulators (TIs) due to their simple surface-state band structures (single Dirac cone) and relatively large bulk band gaps. Nanoscale TI materials are of particular interest as a large surface-to-volume ratio enhances the contribution of surfaces states, meaning they are promising candidates for potential device applications. So far, the vast majority of research efforts have focused on the low-energy (0001) surfaces which correspond to weak planes in the layered crystal structures. Low-dimensional nanostructures (nanowires and nanoparticles) will inevitably involve higher energy facets. We perform a systematic ab-initio investigation of, firstly, the surfaces of bismuth chalcogenide TI nanostructures. These are characterized by different crystallographic orientations as well as local structures and stoichiometries. Secondly, we study the effect of surface orientation on the electronic structure and associated properties of Bi_2Se_3 (Bi_2Te_3) nanostructures. We find several stable surfaces and, depending on the chemical potential value, predict the conditions favouring nanoplate and nanowire morphologies. Surface orientation is found to show a significant effect on the band dispersion and spin polarization of the topological surface-state charge carriers.

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

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Hydrogen (H-) bonds are ubiquitous in nature and play a vital role in, e.g., biological molecules and liquid or solid water. Due to their small mass, H atoms often display pronounced nuclear quantum effects (NQE) such as zero-point delocalisation and quantum tunneling. A powerful method to study NQEs is based on Feynman's path-integrals, where atomic nuclei are treated as ring-polymers. By combining path-integral molecular dynamics (PIMD) with density functional theory (DFT), systems involving breaking of chemical bonds can be treated at a fully ab initio level. Organic H-bonded crystals in the KDP-type family of ferroelectrics display giant isotope effects when D is substituted for H. The ferroelectric-paraelectric phase transition temperature T_c above which these crystals become disordered is shifted by more than 100 K to higher T and geometrical changes of the H-bonds take place. These ferroelectrics are thus both interesting and important to technological applications such as non-linear optics. One member of the KDP-type family of crystals is squaric acid ($C_4H_2O_4$), an anti-ferroelectric layered material with strong in-plane H-bonds and weak inter-plane dispersion interactions. We have performed ab initio PIMD simulations of normal and deuterated squaric acid using DFT functionals including dispersion interactions (vdW functionals) at a range of different temperatures, and compared with classical-nucleus ab initio simulations. While perfect antiferroelectric ordering is seen at all T in classical-nucleus simulations, proton/deuteron jumps are seen to occur at higher T in the PIMD simulations, with a T-dependence mirroring the difference of 150 K in T_c upon deuteration observed experimentally. An elongation of H-bond distances are found in the deuterated crystal, accurately reproducing experiment. Proton/deuteron jumps at higher T are highly cooperative along H-bonding chains and detailed analysis reveals contributions from both thermal activation and quantum tunneling.

Main Topic: A1 Nanoscience

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

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Bromination has been studied extensively since the 1940s as a separation technique for layers in graphite and tubes in nanotube bundles, as well as a highly effective electron acceptor. While many experimental characterisation studies have been performed (notably using Raman spectroscopy), a complete theoretical description of the bromination process and resultant hybrid structures is missing. Notably polybromides such as Br_3^-, Br_5^-, etc have been observed in brominated polymers [1], and there is indirect evidence that such chains may also exist in some brominated carbon nanomaterials (see figure 1).

We present DFT modelling results of bromine in graphene, graphite, isolated and bundled single-walled nanotubes, examining structure, energetics, and also calculating vibrational properties. We identify two key trends for Br_2 behaviour: on graphite surfaces, graphene and outer surfaces of nanotube bundles, Br_2 sits perpendicular to the carbon surface with a vibrational mode ~300cm^{-1}, while between carbon layers it lies parallel to the sheet and auto-arranges, with vibrational mode ~240cm^{-1} [2].

In many cases we find polybromides are more thermodynamically stable than the equivalent Br_2 molecular structures within these carbon materials. These give rise to lower frequency stretch modes at around 170-190cm^{-1}. We propose that these are rarely observed experimentally due to the bromination techniques used, which introduce molecular Br_2 into the carbon host material. Charge transfer with their host material means that these molecules and their associated hole charge in the neighbouring carbon are then coulombically repelled from other bromine molecules, which acts as a barrier to combination into polybromides.

Our calculated barrier for polybromide formation ($2Br_2 \rightarrow Br_4$) in the presence of graphene is 0.35eV .

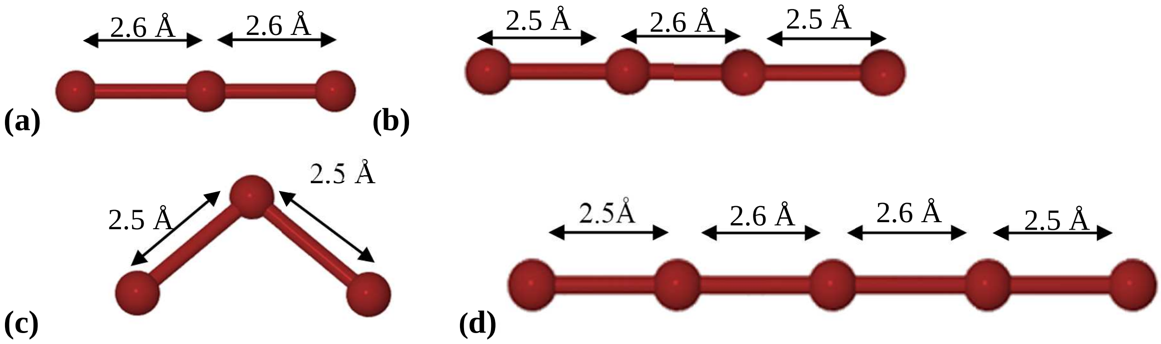

Figure 1. Our optimized geometry of some of the polybromide chains bond lengths with; (a) Br_3^- ($D_{\infty h}$), (b) Br_4^- ($D_{\infty h}$), (c) Br_3^-(C_{2v}), and (d) Br_5^-($D_{\infty h}$) in which the symmetry group of the polybromide chains are given in parenthesis

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Spin crossover induced by an electric bias in nanoscale devices

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Abstract

Manipulation of spin states by physical means is a hot issue in nanoscale materials, due to its potential application in various domains, such as molecular spintronics, display devices, non-linear optics and photomagnetism. Researchers have found that such manipulation (or SCO) can be achieved under external stimuli, such as a change of temperature, application of pressure, light irradiation and even magnetic field. However, it is preferable to achieve this manipulation simply by an electric bias, particularly in the molecular spintronics. This electric SCO would be a great advance in this domain, and more importantly, could provide a useful platform for magnetic molecule-based quantum computing.

In fact, M. Diefenbach & K. S. Tim[1] and N. Baadji & S. Sanvito *et. al.*[2] have proposed a promising mechanism for the electric SCO in isolated molecules, where they concern the distinct difference in response of molecular electronic states upon perturbation with an electric field for different spin states. It is thus our curiosity to figure out this electric SCO in molecular junctions, because that the electron-density redistribution in a molecular junction due to the electrodes and the electric potential drop can greatly influence the response of electronic states upon the perturbation of an electric bias. Eventually, our result by total energy calculation demonstrated that this electric SCO from ferromagnetic coupling of Fe^{2+} ions (FM) to its antiferromagnetic coupling (AF) only existed in the molecular junction of the Fe2(acpypentO)(NCO)3 molecule but was absent in the isolated molecule. This result implies that this SCO absent in an isolated molecule could be achieved in its molecular junction. We have also provided evidences of that the electrodes and the electric potential drop in a molecular junction really have substantial effect on this electric SCO[3].

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

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Graphene is a very promising material for a large variety of applications due to its singular properties. These properties can be modified by defect formation in the sample, thus the study of these formations could help to control the properties of graphene.

Andrey Chuvilin has observed by TEM that in bilayer graphene under electron radiation one type of defect, called butterfly defect, is formed for lower electronic energies than the displacement threshold energy for monolayer graphene. Our first objective has been to analyse using the SIESTA method, based on first principles calculations, the equilibrium state in the low-temperature limit of the monolayer and bilayer graphene system containing the butterfly defect. Thus, we have been able to observe the influence that the addition of the second layer has on the energy and geometry of the system.

Although we observed that the presence of the butterfly defect in the bilayer graphene is energetically more favorable with respect to the mono-layer graphene, the energy difference is small $\sim$0.1 eV, not enough to explain Chuvilin's observations. The deformations caused by the presence of the defect in the bilayer graphene are very small, which is consistent with the fact that there is not any new strong interaction between the layers.

Finally, we are making a kinetic analysis based on molecular dynamics of the system because we think that the observed effect will be of kinetic origin.