Title: **Water on graphene oxide: steps toward understanding ultrafast proton transport theoretically**

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Abstract:

The phenomenon of proton transport has relevance to diverse areas such as biological systems, sensors and fuel cells. For fuel cell applications, conduction through the electrolyte can occur via proton transport. Ideally, the electrolyte should conduct well under humid and hot conditions, graphene oxide promises to be such a material. It has been shown experimentally that the conductivity of a single layer graphene oxide increases almost linearly from 6 x 10 -7 S cm -1 at 55 % relative humidity (RH) to 2 x 10 -4 S cm -1 at 90 % relative humidity. The conductivity also increases with the film thickness. In this study, we use ab initio density functional theory and ab initio molecular dynamics to study the behaviour of water on a single sheet of graphene oxide. In particular, we study the contrasting behaviour of water molecules on hydrophobic and hydrophilic regions of graphene oxide, and the formation of water bridges that link hydrophobic patches to one another. We also gain clues toward understanding the fast proton transport by plotting the energy landscape as a proton is transferred across various regions of the water on graphene oxide system.

Title: **Stability of Pt-Ru alloy for anode catalyst and CO tolerance mechanism in PEFC Fuel Cell using combined DFT and Monte Carlo Simulation**

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Department of Natural Sciences
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Abstract:
Pt-Ru alloys are known to substantially improve the catalytic performance in the electrochemical oxidation of CO from CO contaminated hydrogen fuels. The CO itself is usually assumed to follow a so-called bifunctional mechanism, originally suggested by Watanbe and Motoo. For H2 oxidation in the presence of CO, Watanabe and Motoo have proposed a combined mechanism, in which the ligand and bifunctional effects may coexist. The improvement of the catalytic performance requires an understanding of the reaction mechanism at the atomistic level. Initially, we have checked the surface stability of Pt-Ru surface with different positions of Pt and Ru remaining same mixing ratio. We found that fcc based Pt-Ru alloy shows higher stability than the hcp based alloy and we also confirmed that the surface coverage with Pt atoms indicates stable combination. As a whole the tendency indicates, top surface contains Pt sufficiency and 2nd layer contains Ru sufficiency make the structure stable. Many studies assumed that Pt-metal alloy shows more reactivity than pure Pt for CO oxidation but very few studies regarding atomistic level. MC simulations further study coverage change of Pt on the surface of alloy catalysts. Based on the DFT calculations I correlate the binding energy of alloy catalysts with different Pt coverage. We performed MC simulation in the presence of gases (H2,CO). From our MC simulation study I successfully modeled the temperature effect on Pt-Ru alloy surface change as well as CO poisoning influence to Pt coverage of this bimetallic surface.

Title: **Physical adsorption: Nanoscale van der Waals interactions beyond the Lifshitz-Zaremba-Kohn limit**

Alberto Ambrosetti
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Abstract:
The Lifshitz-Zaremba-Kohn (LZK) theory is commonly considered as the correct large-distance limit for the van der Waals (vdW) interaction of adsorbates (atoms, molecules, or nanoparticles) with solid substrates. The LZK approach predicts universal power laws for vdW interactions depending only on the dimensionality of the interacting objects. However, recent experimental findings are challenging the universality of the LZK theory at finite distances of relevance for nanoscale assembly. Here, we present a combined analytical and numerical many-body study demonstrating that physical adsorption can be significantly enhanced at the nanoscale. Regardless of the band gap or the nature of the adsorbate specie, we find deviations from conventional LZK power laws that extend to separation distances of up to 10--20 nanometers. The sensitivity of vdW interactions to the substrate response and to the adsorbate characteristic excitation frequency suggests that adsorption strength can be effectively tuned in experiments, paving the way to an improved control of physical adsorption at the nanoscale.

Title: **Giant magnetoelectricity in Ni3TeO6 from first principles**

Sergey Artyukhin
Italian Institute of Technology
Quantum Materials Theory group
Genova, Italy

Abstract:

principal collaborators: S.-W. Cheong, D Vanderbilt, K Haule (Rutgers U) V. Zapf (LANL) J Musfeldt (U Tennessee, Knoxville)
the poster presents the work from the publictaions [1-3]

[1] Colossal magnetoelectricity in a collinear antiferromagnet Ni3TeO6,
Y.-S. Oh, S. Artyukhin J. J. Yang, V. Zapf, J.-W. Kim, D. Vanderbilt, S.-W. Cheong,
Nature Communications 5, 3201 (2014)
[2] Successive magnetic-field-induced transitions and colossal magnetoelectric effect in Ni3TeO6,
J.W. Kim, S. Artyukhin, E. D. Mun, M. Jaime, N. Harrison, A. Hansen, J. J. Yang, Y. S. Oh, D. Vanderbilt, V. S. Zapf, and S.-W. Cheong,
Phys. Rev. Lett. 115, 137201 (2015)
[3] Magnetoelectric coupling through the spin flop transition in Ni3TeO6, M.O. Yokosuk, A. al-Wahish, S. Artyukhin, K.R. O'Neal, D. Mazumdar, P. Chen, J. Yang, Y.S. Oh, S.A. McGill, K. Haule, S. Cheong, D. Vanderbilt, and J.L. Musfeldt, Phys. Rev. Lett. 117, 147402 (2016).

Title: **Anharmonicity and the isotope effect in superconducting lithium at high pressures: a first-principles approach**

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Abstract:

Recent experiments (A. M. Schaeffer, Proceedings of the National Academy of Sciences 112, 60 (2015)) have shown that lithium presents an extremely anomalous isotope effect in the 15-26 GPa pressure range. In this work we have calculated the anharmonic phonon dispersion of ^{7}Li and ^{6}Li under pressure, their superconducting transition temperatures and the associated isotope effect. We have found a huge anharmonic renormalization of a transverse acoustic soft mode along ΓK in the fcc phase, the expected structure at the pressure range of interest. In fact, the anharmonic correction dynamically stabilizes the fcc phase. However, we have not found any anomalous scaling of the superconducting temperature with the isotopic mass. Additionally, we have also analyzed whether the two lithium isotopes adopting different structures could explain the observed anomalous behavior.

Title: **Electronic and Optical properties of hydrogenated TiO2**

Samaneh Ataei Seyedeh
University of Tehran
Department of Physics
Tehran, Iran

Abstract:
We have studied the electronic and optical properties of hydrogenated Tio2 using spin polarized DFT+U calculations with Quantum espresso code.

Title: **First Principle Calculations of LiRh2Ge and LiCu2Ge Heusler Alloys**

Seyfettin Ayhan
Graduate School of Natural and Applied Sicence
Diyarbakır, Turkey

Abstract:

Structural, elastic, electronic and magnetic properties of the huesler phase LiRh2Ge and LiCu2Ge are investigated using ab initio technique as implemented in self- consistent full-potential linearized augmented plane wave (FPLAPW) method Perdew, Burke and Ernzerhof (PBE) 96 generalized gradient approximation. The computed equilibrium lattice parameters for the compounds are in good agreement with previous theoretical result and experimental data. The elastic constants reveal that the compounds are elastically stable.

Title: **Ab-initio Raman spectroscopy within the DFPT+PAW formalism**

Lucas Baguet
CEA, DAM, DIF
Arpajon, France

Abstract:

The interpretation of experimental Raman spectra of materials is, in general, a difficult task. To compare these spectra with theoretical ones gives a deeper understanding of the underlying physical phenomena.
The computation of theoretical Raman spectra requires the third-order derivatives of the ground state energy, which can be done using the $2n+1$ theorem, as in the Density Functional Perturbation Theory (DFPT), or with finite difference methods. Existing works using the $2n+1$ theorem are limited to norm-conserving (NC) (as in Veithen et al, Phys. Rev. B 71, 125107 (2005)) or ultra-soft (US) pseudo-potentials (Miwa, Phys. Rev. B 84, 094304 (2011)).
We present a method adapted to the projector-augmented wave (PAW) formalism, which conciliates the small cost of NC pseudo-potentials with the precision of all-electron calculations. Contrary to Veithen et al, the electric field perturbation is treated analytically, leading to the resolution of a second-order Sternheimer equation (as in the work of Miwa). Comparing the different approaches, our results show that the analytical one has the best k-point convergence.

Title: **One-shot calculation of complete low pressure phase diagrams.**

Robert Baldock
EPFL, School of Engineering
Institute of Materials
Theory and Simulation of Materials
Lausanne, Switzerland

Abstract:
We present a new nested sampling algorithm that allows the calculation of complete pressure temperature phase diagrams below 1 GPa in a single calculation. The new algorithm yeilds the partition function as an explicit function of both pressure and temperature. Higher pressures can be achieved by additional fixed-pressure calculations, which can be interpolated using a reweighting technique also described in this poster. We demonstrate the approach by calculating the low-pressure phase diagram of the Lennard-Jones system.

Title: **High-throughput screening of binary oxides to discover intermediate band compounds**

Douglas Baquião Ribeiro
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Santo André, Brazil

Abstract:

Intermediate band existence in semiconducting materials indicates a series of potential applications to devices, from supercapacitors and memristors to solar cells. In this work, our focus was to create a descriptor capable of searching in the AFLOWlib-ICSD materials database for compounds that would fit in the classification of intermediate band materials. The chosen ones were those materials that showed at least one narrow band (maximum of 1 eV) next to the energy gap, considering this to be a region with 3 eV of maximum distance to the Fermi level. After that, it was built a periodic table representation indicating successful combinations of oxygen with 32 elements, considering the initial spectrum of more than 55,000 compounds and, after the descriptor action besides post-processing analysis, it was possible to achieve a collection of 333 materials. Using these results, we continued to the next stage of project, which consisted in selecting some of these compounds to be charged, adding or subtracting electrons.

Title: **Ab initio study of structural, electronic and hydriding properties of FeTi intermetallic**

BENTAYEB Fatima-Zohra
Physics Department
Annaba, Algeria

<u>Abstract</u>:
In this work, ab initio study of hydrogen storage in FeTi intermetallic is carried out. Structural and electronic properties of TiFeH and TiFeH2 hydrides with orthorhombic structure are investigated by means of the self-consistent SIESTA code. Total energies, atomic forces and stresses are calculated by solving the electronic quantum-mechanical equation using the density functional (DFT) approach in the generalized gradient approximation (GGA). Lattice parameters, bulk modulus and electronic structure are investigated in the ground state. The cell parameters and atomic coordinates are fully relaxed by the conjugate gradient optimization. The DOS and band structure analysis show that the mono- and di-hydrides have metallic behaviour. The obtained results are in good agreement with experimental data and previous theoretical studies.

Title: **A first-principles study of liquid and amorphous phases of the In2Te3 compound**

Marco Bernasconi
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Dip. Scienza dei Materiali
Milano, Italy

Abstract:
Phase-change materials have been widely used in electronic industry thanks to their ability to rapidly and reversibly switch from amorphous to crystalline phase. In par- ticular, being a good compromise between speed of crystallization and stability of the amorphous phase, Ge2Sb2Te5 proved to be an excellent material for optical-storage de- vices such as DVD and non-volatile phase-change memories (PCMs). Despite its success though, the crystallization temperature of this compound (≈ 393 K) is too low for ap- plications in automotive where higher working temperatures are required. Hence, the necessity to find new materials which crystallize at higher temperatures. Along this direction, the ternary system In-Sb-Te has been proposed as a possible alternative can- didate. In order to better understand the properties of the ternary system we decided first to take under consideration the In-Te compound, focusing our attention on the In2Te3 composition. Using molecular dynamics based on density functional theory we perform a comprehensive study of the structural, vibrational and electronic properties of the liquid and of the glass quenched from the melt. We compare results obtained with BLYP and BLYP+D3, rVV10 which also include van der Waals interactions. We observe that all the models show a mostly tetrahedral environment for In atoms and a mostly pyramidal configuration for Te atoms, similarly to the local geometry of the crystalline phase.

Title: **B1-B2 phase transition of LiH at finite temperature**

Sananda Biswas
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India

Abstract:

Lithium hydride (LiH) is a promising candidate for a hydrogen storage material and it is currently used in various industrial applications such as in hydrogen generators and in the ceramic manufacturing. LiH is the most elementary ionic crystal, having only four electrons per primitive unit cell. At ambient conditions, it crystallizes in the B1 (NaCl) structure and is a large-gap insulator. Previous theoretical studies suggest that LiH undergoes a phase transition from B1 to B2 (CsCl structure) at high pressure. The transition was suggested to be accompanied by a softening of the transverse acoustic phonon mode at the zone boundary X point of the Brillouin zone. This phase transition was suggested to be accompanied with insulator-metal phase transition of the system. Previous theoretical studies had suggested the transition pressure to vary between 85 to 450 GPa at low temperature. Recent diamond-anvil cell experiments up to 252 GPa did not observe any transition at room temperature. However, recent shock-wave experiment suggests a B1-B2 transition pressure of 120 GPa at 1800 K, suggesting that the B1-B2 transition could be strongly temperature dependent. This unusual behavior may be attributed to the anharmonic effects to the vibrational free energy, which has been neglected so far. Here we have studied the temperature dependence of the B1-B2 transition pressure of LiH, taking into full account the anharmonic contribution to the free energy via a recently developed method called stochastic self-consistent harmonic approximation (SSCHA).

Title: **Quasiparticle band structure and optical properties of hexagonal-YMnO3**

Tathagata Biswas
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Department of Physics
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India

Abstract:
We use the first principles methods to study the electronic structure and optical properties of G-type anti-ferromagnetic hexagonal-YMnO3. Hexagonal-YMnO3 is a multiferroic, which has been found to be a ferroelectric below 914 K and also has anti-ferromagnetic order with a Neel temperature of 80 K. We calculate ground state properties of this material within density functional theory (DFT) using the DFT+U formalism. We calculated the quasiparticle band structure of this material using many body perturbation theory within the GW approximation. In order to understand the optical response of this material, we solved the Bethe–Salpeter equation and calculated the absorption spectrum. Our calculated optical band gap of 1.45 eV agrees well with the experimental value of 1.55 eV. We find an exciton binding energy of 0.21 eV for this material. Our calculation reveals that the exciton in this material has a strong bidimensional character, localized in the plane containing Mn and O. Although the relatively large exciton binding energy makes it difficult to use it in most of the photovoltaic applications, this bidimensional character can open up interesting optical applications utilizing surfaces of this material in nanostructures.

Title: **Anharmonic enhancement of superconductivity in molecular hydrogen at high pressure**

Miguel Borinaga
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Abstract:
First-principles calculations based on density-functional theory including anharmonicity within the variational stochastic self-consistent harmonic approximation are applied to understand how the quantum character of the proton affects the candidate metallic molecular Cmca − 4 structure of hydrogen in the 400–450 GPa pressure range, where metallization of hydrogen is expected to occur. Anharmonic effects, which become crucial due to the zero-point motion, have a large impact on the hydrogen molecules by increasing the intramolecular distance by approximately a 6%. This induces two new electron pockets at the Fermi surface opening new scattering channels for the electron–phonon interaction. Consequently, the electron–phonon coupling constant and the superconducting critical temperature are approximately doubled by anharmonicity and Cmca − 4 hydrogen becomes a superconductor above 200 K in all the studied pressure range. Contrary to many superconducting hydrides, where anharmoncity tends to lower the superconducting critical temperature, our results show that it can enhance superconductivity in molecular hydrogen.

Title: **Mechanistic study of zeolite -catalysed dehydration of ethanol to ethylene (formation of the likely precusor for hydrocarbons.)**

Cecil Botchway
Kwame Nkrumah University of Sceince and Technology
Kumasi, Ghana

Abstract:
The mechanism of conversion of ethanol to ethylene over the zeolite catalyst FER has been studied at the density functional theory level with the QUANTUM ESPRESSO code. The adsorption of the ethanol which is the first step to the reaction, depends sensitivity on the Si/Al ratio of the zeolite. The most stable adsorption site on the on the zeolite was found to be on the Si/Al ratio of 5 which is configuration of the natural zeolite ferrierite and the least stable site were found on the ratio 8. The reaction energies of the product yielded ethylene and water were found to be in the ranges of 4- 14 kcal/mol .

Vacancy in graphene nano-flakes: a first principles study

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Graphene nano-flakes GNFs present interesting properties [1] that differ from those of extended graphene. It is well known that the electronic and magnetic properties of model, ideal GNFs depend crucially on the geometry of the edges [2]. In this perspective, already pristine GNFs can have nonzero spin magnetic moment due to the sub-lattice imbalance [3-5]. On the other hand, the single vacancy in 2-D graphene has been proposed to give rise to magnetism [6], and it is thus interesting to investigate the character obtained for this defect in a GNF.

We here present a theoretical study of a single vacancy in different GNFs, with planar hexagonal H or trigonal T shapes, with armchair AC or zigzag ZZ edges, passivated with hydrogen atoms. We work within Density Functional Theory DFT employing the Perdew-Burke-Ernzerhof functionals DFT and hybrid DFT&Hartree-Fock (PBE and PBEh) [7-9]. All calculations are performed using the all-electron FHI-aims code with spin-polarization [10,11].

We start our discussion with results for perfect GNFs. As expected, we find that TZZ flakes have an intrinsic spin due to the sub-lattice imbalance, whereas in the H flakes such imbalance does not exist, and the spin is zero. Passing to the vacancy, the formation energy is ~7.6 eV in the different GNFs, in agreement with earlier theoretical results [12-14]. We point out that, for H-GNFs, taking one C atom out creates a sub-lattice imbalance: indeed, we find magnetic character for the vacancy already with PBE functional. T in his is not the case for TZZ-GNFs, where the formation of the defect just alters the imbalance. We stress that now the inclusion of exact-exchange is required to obtain non-zero spin magnetic moment. In conclusion, also in agreement with earlier work [15], for all GNFs we simulated, using hybrid DFT we find that the vacancy induces a magnetic moment of $2\mu_B$.

[1] C. Cocchi et al, *J. Phys. Chem.* A **118**, 6507 (2014); [2] S. Fujii and T. Enoki, *Acc. Chem. Res*. **46**, 2202 (2013); [3] W. Wang et al., *Nano Lett.* **8**, 241 (2008); [4] J. Fernández-Rossi and J.J. Palacios., *Phys.Rev.Lett*. **99**, 177204 (2007); [5] E.H. Lieb, *Phys. Rev. Lett.* **62**, 1201 (1989); [6] J. Palacios and F. Ynduráin. *Phys. Rev. B* **85**, 245443 (2012); [7] J.P. Perdew, M. Ernzerhof and K. Burke, *Phys. Rev. Lett.* **77**, 3865 (1996); [8] J.P. Perdew et al., *J. Chem. Phys.* **105**, 9982 (1996); [9] M. Pinheiro et al., *Phys.Rev.B.* **92**, 195134 (2015); [10] V. Blum, et al., *Comput. Phys. Comm.* **180**, 2175 (2009); [11] A. Tkatchenko and M. Scheffler, *Phys. Rev. Lett.* **102**, 073005 (2009); [12] A.A. El-Barbary, et al. *Phys.Rev.B.* **68**,144107 (2003); [13] A. Krasheninnikov, et al. *Chem.Phys. Lett.* **418**, 132 (2006); [14] S.T. Skowron et al. *Chem. Soc. Rev.* **44**, 3143 (2015); [15] B. Wang, and S. T. Pantelides, *Phys. Rev. B.* **86**, 165438 (2012).

Title: **Doping, co-doping, and defect effects on the plasmonic activity of ZnO-based transparent conductive oxides**

Arrigo Calzolari
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Abstract:
Using simulation from first principles we investigate the role of doping, co-doping and point defects on the optoelectronic properties of metal-doped ZnO (MZO), as transparent conductive oxide for energy applications. Further we study the plasmonic activity of MZO in the near-IR range and in particular at wavelength relevant for telecommunications (1,5 μm), in agreement with the experimental results.

Title: **Computational design of novel 2d-materials for electronic applications**

Davide Campi
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Abstract:
Novel materials are at the basis of the future progress in information-and-communications technologies (ICT) and in energy harvesting, conversion, and storage. 2D materials present an entire novel paradigm and toolbox for materials scientist to discover new properties and functionalities. In absolute terms however, the handful of 2D materials intensively studied up to now represent only the tip of an iceberg. In this work we present the preliminary results of an applications-oriented screening that, using state-of-the-art first-principles simulations and automatized high-throughput calculations, aims at identifying the most promising candidates among the hundreds of new 2D materials discovered by performing a "computational exfoliation" of a dataset of more than 200000 bulk parent structures. The possible performances of each material in different electronic applications are evaluated using figures of merit based on descriptors like the band gap, effective masses, workfunction and acoustic phonon limited mobility.

Title: **ATOMIC SCALE INVESTIGATION OF GRAPHENE MOIRE' STRUCTURES ON NI(100)**

Virginia Carnevali
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Department of Physics
Trieste, Italy

Abstract:

Graphene on Ni(100) forms a variety of Moire' patterns which can be well explained in atomistic models by the mismatch with the substrate, with periodicity depending on the relative angle between the hexagonal graphene and the square surface lattices. Evidence of the different Moire' structures is given by high resolution scanning tunneling microscopy images, that are well reproduced by ab-initio simulations. Beyond providing the detailed atomic-scale structures, the numerical simulations allow a deep local characterization of the chemical bonding between the graphene layer and the support. We also discuss the possible formation beneath the graphene of a surface-confined nickel- carbide in specific regions of the Moire', whose presence is suggested by experimental STM images.

Title: **Ab-initio molecular dynamics simulations of polaron- and exciton-induced OLED degradation**

Marco Cazzaniga
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Consiglio Nazionale delle Ricerche, CNR
Milano, Italy

Abstract:
Organic light-emitting diodes (OLEDs) offer the potential of using both the singlet and triplet excitons in realizing 100% internal quantum efficiency of electro-luminescence. However, the injected charge carriers (electrons and holes) may become trapped at morphological and chemical defects, and recombine non-radiatively. These phenomena, not only limit the quantum efficiency of the device, but are also responsible for its degradation (leading to aging and failure), through the formation of highly reactive radical species. A complete understanding of the degradation pathways, beyond phenomenological models, based on atomistic/microscopic modeling, is still missing to date. We performed Car-Parrinello molecular dynamics with constrained orbital occupations to simulate the fate of an electron, a hole and an electron-hole pair, electrically injected into the device. We address few molecules used in OLEDs both as host material (CBP aNPD and mCP) and as phosphorescent emitter (FIrpic). We found that polaron- and exciton-trapping can induce large conformational changes, the weakening of some ancillary bonds and in the worst case the dissociation of some fragments of the molecule.

Title: **Organic functionalization of MoS2 monolayer**

Giancarlo Cicero
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Torino, Italy

Abstract:

Recently 2D layered materials based on transition metal dichalcogenides (TMD) have received a large amount of attention because of their peculiar and versatile physical properties. Mono and few-layered TMDs are direct-gap semiconductors whose band gap energy, as well as carrier type varies depending on the composition, structure and dimensionality of the system. In particular MoS2 has been proposed as active absorbing layer in photovoltaic application due to its efficient absorption in the visible energy range but also as photocatalyst for hydrogen evolution reaction. The efficiency of MoS2 in this kind of applications depends on the ability of this material to absorb part of the visible spectra but also on the spatial localization of the electron/hole pair upon excitation. Moreover it would be important to be able to tune the conductivity of the MoS2 monolayer by accurately modifying its structure.

Here we present theoretical predictions of the electronic and optical properties of MoS2 modified with different organic molecules, namely methyl and thiophene derived compounds. In our work, the equilibrium structures of the hybrid MoS2/organic systems are obtained by means of ab initio density functional theory simulations, while absorption spectra are calculated employing the GW-Bethe Salpeter method. The proposed molecules are found to chemically bind to the T' phase of MoS2 monolayer and not to the H one, inverting the stability of the two unmodified phases. Our results show that the proposed molecules are able to strongly modify the electronic properties of the MoS2 monolayer and effectively tune its the absorption spectra.

Title: **Koopmans-compliant functionals: A reliable and efficient tool for spectroscopic quantities.**

Nicola Colonna
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Abstract:
In exact density-functional theory the total energy as a function of the particle number is a piecewise-linear sequence of straight lines connecting integer points. However, commonly used approximate density functionals produce total energies that do not exhibit such piecewise-linear behaviour, leading to a discrepancy between total and partial electron removal/addition energies and poor predictive capabilities of ionization potentials. Koopmans-compliant functionals enforce a generalized criterion of piecewise linearity in the energy of any approximate density functional with respect to the partial removal/addition of an electron - i.e., with respect to charged excitations - from/to any orbital of the system. When used to purify approximate density functionals, Koopmans' corrections lead to orbital-density dependent functionals and potentials that are able to deliver accurate spectroscopic properties. The approach has been benchmarked on a comprehensive variety of molecular systems for which high accuracy calculations are available: the G2-R1 set, organic donors and acceptors, DNA/RNA bases, and transition-metal complexes. Results for ionization potentials, electron affinities, and photoemission spectra are typically comparable, but slightly superior, to those obtained with different flavours of GW many-body perturbation theory. Being this a functional framework, the straightforward advantages are that forces and other derivatives are also readily accessible, that the computational costs are much reduced, and the numerical parameters are those typical of DFT total-energy calculations. Applications of the Koopmans' functionals to extended systems are also discussed, again showing very good agreement with experiments or higher-order theories.

Title: **Thermal energy storage in nanofluids: what can simulations teach us?**

Francesca Costanzo
Cataln Institute of Nanoscience and Nanotechnology
Barcelona, Spain

Abstract:

Ionic Liquids are one of the preferred options used by the industry for the storage of thermal energy in solar energy plants. Improving their thermophysical properties is an important goal to achieve more efficient heat storage and transportation media. A promising approach for improving these properties is to introduce nanoparticles dispersed in the ionic liquid or the molten salt, the so-called nanofluids. However, how thermophysical properties such as the heat capacity, self-diffusion, or heat conductivity depend on the microstructure of the nanofluids is still rather unknown. Molecular simulation, therefore, can play a major role in this research, as producing reliable experimental data for these systems is difficult and expensive. We have calculated by classical molecular dynamic simulations, thermal properties of disk-like graphene nanoflakes dispersed in organic solvent. In my contribution, I will discuss how the heat capacity and the thermal conductivity depend on the shape, the size and the density of the dispersed carbon nanoflakes. With our classical model, we are able to shed light and gather basic understanding on the dependence of thermal transport properties on the nature of solute-solute and solute-solvent interaction.

Work supported by the MaX Center of Excellence in HPC Applications (http://www.max-centre.eu/), financed by EU Grant H2020-676598.

Title: **Graphene-based synthetic antiferromagnets: an ab-initio study**

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Abstract:
By means of atomistic first principles calculations we have undertaken a structural, electronic and magnetic study of Fe/Gr/Co/Ir(111) hybrid graphene/magnetic structure using SIESTA DFT package [1]. These kind of materials play a fundamental role in emerging graphene spintronic technologies such as those based in room-temperature long-spin lifetimes or tunnel magneto-resistance [2]. The Fe-to Graphene/Co/Ir binding mechanisms were investigated via the adsorption energy, charge transfer, density of states, and hybridisation analysis. We show theoretically that a strong perpendicular antiferromagnetic coupling can be established in ultrathin-film structures such as Fe/Gr/Co on Ir(111). To this respect Graphene acts not only as a mere spacer but has a direct role in sustaining antiferromagnetic superexchange-coupling between the Fe and Co magnetic layers by means of the hybridisation between Co-3d and Gr's pz states. In addition, the calculated magnetocrystalline anisotropy values are in good agreement with the experiments.

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[2] V. M. Karpan, G. Giovannetti, P. A. Khomyakov, M. Talanana, A. A. Starikov, M. Zwierzycki, J. van den Brink, G. Brocks, and P. J. Kelly, Physical Review Letters 99, 176602 (2007).

Title: **Symmetry classification of the electronic states and of the normal vibrational modes of a solid using the projective representations of the point group: a numerical implementation**

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Abstract:
We present a numerical implementation of a classification method for the analysis of the symmetry of the one-electron Bloch wave-functions and of the phonon modes of solids with non symmorphic space groups at the Brillouin zone border, based on the projective irreducible representations of the small point group of the wave-vector.[1] We illustrate the method with the classical examples of application to the symmetry classification of electronic band structure of Silicon (space group $Fd\bar3m$). The symmetry of both the scalar relativistic and of the fully relativistic Bloch wave-functions are discussed at the relevant points and lines of the Brillouin zone. Finally we discuss the symmetry properties of the phonon modes of hexagonal close-packed Beryllium at zone border (space group $P6_3/mmc$).

[1] S. K. Kim, Group theoretical methods and applications to molecules and crystals, Cambridge University Press (1999).

Title: **X atoms inserted in hematite photoanodes for enhancing photoelectrochemical activity: An ab initio prediction**

Bruno Dandogbessi
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Abuja, Nigeria

Abstract:
The structural and electronic properties of hematite doped with atoms X were systematically investigated using ab initio calculations. We found that the structural changes and the atomic radii of the doped X atoms are responsible for remarkable decreases in band gap, which enhance the absorption coefficients of photons.

Title: **Machine-learning based interatomic potential for amorphous carbon**

Volker Deringer
University of Cambridge
Department of Engineering and Department of Chemistry
Cambridge, United Kingdom

Abstract:

We have developed a Gaussian approximation potential (GAP) model for atomistic simulations of liquid and amorphous carbon. GAP is a machine-learning based approach to enable development of interatomic potentials, in which a large database of DFT-computed energies and forces is used to generate a high-dimensional fit to the potential-energy surface. On this poster, I will introduce our new GAP model, describe its energy and force accuracy as well as structural "benchmarking" against DFT reference data, and present exemplary applications to surfaces of tetrahedral ("diamond-like") amorphous carbon. This new interatomic potential appears to be promising for large-scale atomistic modelling of amorphous carbon structures.

Title: **Strong correlation in Double-Perovskites using DFT+U**

DJERMOUNI Mostefa
University Djilali Liabès of Sidi Bel-Abbès
Sidi Bel-Abbès, Algeria

Abstract:
A Density functional theory (DFT) based on LAPW basis set have been carried out on crystalline bulk double perovskites Sr2TiCoO6 in order to determine and correlate their structural, electronic and magnetic properties. The crystallographic structure evolves from cubic to tetragonal, and the electronic structure changes from "Anti-ferromagnetic Insulator" to "Ferromagnetic Half-metal".

Title: **Gaussian approximation potentials for α-iron**

Daniele Dragoni
Universita' degli Studi di Milano - Bicocca
Dipartimento di Scienze dei materiali
Milano, Italy

Abstract:

Interatomic potentials are often necessary to describe complex realistic systems that would be too costly to study from first-principles. Commonly, they are designed using functional forms driven by physical intuition and fitted to experimental or computational data. The moderate flexibility of these functional forms limits their ability to be systematically improved by increasing the fitting datasets; on the other hand, their qualitative description of the essential physical interactions ensures a modicum degree of transferability. Recently, a novel trend has emerged where potential-energy surfaces are represented by neural networks fitted on large numbers of first-principles calculations, thus maximizing flexibility but requiring extensive datasets to ensure transferability. Gaussian Approximation Potentials in particular are a novel class of potentials based on non-linear, non-parametric Gaussian-process regression. We apply here this approach to the case of alpha-iron, training a GAP model from energies, stresses and forces taken from first-principles molecular dynamics simulations of pristine and defected bulk systems, of surfaces and gamma-surfaces with different crystallographic orientations, covering more than 10^5 local atomic environments. We verify this GAP model by comparing its predicted structural, vibrational, and thermodynamic properties against those derived directly from first-principles and prove that, thanks to a meticulous control on the database generation, it is possible to train models which can achieve plane-waves density functional theory accuracy.

Title: **A downfolded effective Hamiltonian combining MBPT with quantum chemistry**

Dvorak Marc
Aalto University
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Abstract:

We present a new method to predict optical excitations and ionization energies in correlated systems. Focusing on molecules here, we first partition the many-electron Hilbert space into a weakly correlated, high-energy subspace and a correlated, low-energy subspace that contains the relevant excitations. Correlation between the two spaces is treated with many-body perturbation theory (MBPT), allowing us to downfold the effect of the high-energy space onto an energy dependent effective Hamiltonian for the low-energy space [1]. This effective low-energy Hamiltonian is diagonalized with configuration interaction (CI). The main effect of the downfolding procedure is to introduce corrections to the ordinary CI Hamiltonian based on the screening of the Coulomb interaction in the low-energy subspace by high-energy electronic transitions. At zeroeth order, this procedure gives the familiar frozen core approximation. However, we expand the corrections to infinite order with the constrained random phase approximation (cRPA), generating new two-body corrections to the normal CI Hamiltonian. In this way, we treat weakly correlated states with MBPT and strongly correlated electrons with our chosen level of CI. Our downfolded method is a new route to highly accurate, efficient calculations of excitations in moderate sized molecules.

1. V. A. Dzuba, V. V. Flambaum, and M. G. Kozlov, Phys. Rev. A 54, 3948 (1996).

Title: **Competing Structures in (In,Ga)Se and (In,Ga)2Se3 Semiconductors**

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Department of Physics
Laboratoire de Physique et d'Electroninque (LPE)
Beirut, Lebanon

Abstract:
The electronic structure of four polytypes (Beta, Gamma, Delta and Epsilon) of hexagonal GaSe and InSe is calculated from first principles, using the WIEN2k and VASP codes and PBEsol prescription for the exchange-correlation potential, aiming specifically at elucidating the crystallographic parameters and comparing the energy placement of corresponding competing structures. Further on, the compounds with different composition of the same constituents, namely the ordered-vacancies systems Ga2Se3 and In2Se3, were subject to a similar study, of which the relaxed crystal structure data for three different phases is reported. Comparison is done with the nominal wurtzite structure over which the cation vacancies are introduced, and the relaxation pattern discussed.

Title: **Ab initio quality neural network potential for CaF2 based on charge equilibration process**

Somayeh Faraji Nafchi
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Zanjan, Iran

Abstract:
This work presents the development of machine learning based potential for CaF2 compound. Training data set includes only CaF2 cluster structures. The potential can describe the fundamental physical properties of CaF2, including cohesive energy, elastic constants, surface energies and phonon properties of CaF2 comparable to that obtained from first-principles calculations through LDA and PBE exchange correlation functionals. Actually, we demonstrate that the results of the cluster-trained neural network potential reproduces PBE results with an error less than or comparable with the difference between LDA and PBE exchange correlation functionals.

Title: **Toward the non-equilibrium Green's function calculation based on a divide-conquer approach**

Mashiro Fukuda
Institute for Solid State Physics
University of Tokyo
Ozaki Laboratory
Chiba, Japan

Abstract:
We propose a linear scaling non-equilibrium Green's function (NEGF) method based on a divide-conquer (DC) approach with a correction by self-energy terms, whose computational cost scales only linearly. The NEGF method combined with density functional theory has been proven to be a useful tool to investigate electronic transport properties of nanoscale materials such as spin filtering devices and topological insulators. However, its further applications to more realistic models consisting of, e.g., multi-electrodes, scattering regions, substrates, and multi-gates are still very challenging issues due to the cubic scaling in the computational cost. To apply the NEGF to realistic models, we propose a linear scaling NEGF method based on a DC approach, which allows us to tackle large-scale systems. However, applying the DC approach to the NEGF method simply can make it hard to obtain converged results due to the influence of the dangling bonds of a truncated cluster, even though the size of the truncated cluster is large. In order to avoid the convergence problem we include the effect of the dangling bonds approximately by using the self-energy which is given by Green's functions of neighboring atoms of the truncated cluster. We show that this scheme can give sufficient accuracy to the transmission calculations by using a programcode OpenMX(http://www.openmx-square.org/).

Title: **Structural Relaxations and Resistance Drift in Amorphous GeTe from Atomistic Simulations**

Silvia Gabardi
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Milano, Italy

Abstract:
Tellurium-based chalcogenide phase change alloys have been recently investigated because of their use in optical (DVD) and electronic (phase change memories, PCM) data-storage devices. Both applications rest on the fast (10-100 ns) and reversible transformation between the crystalline and amorphous phases induced by heating. The two states of the memory can be discriminated thanks to the large difference in optical reflectivity and electronic conductivity of the two phases. While the crystal is stable at normal conditions, the amorphous is subject to structural relaxations with time.

This aging process is a common feature of the glassy state which in the case of phase change chalcogenide leads to an increase of the electrical resistance with time. This phenomenon called drift is detrimental in the application of these materials in PCMs. By means of combined molecular dynamics and electronic structure calculations based on density functional theory we have unravelled the atomistic origin of the resistance drift in the prototypical phase change compound GeTe. 2000-atom models of amorphous GeTe have been generated by quenching from the melt by means of molecular dynamics simulations based on a Neural Network potential. The aging process has been mimicked either by annealing or by metadynamics simulations.

The drift results from a widening of the band gap and a reduction of in-gap states due to structural relaxations leading to the removal of chains of Ge-Ge homopolar bonds. The same structural features are responsible for the high mobility above the glass transition which boosts the crystallization speed exploited in the device.

Title: **One-dimensional metallic wires at phase-engineered boundaries in two-dimensional materials**

Marco Gibertini
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Lausanne, Switzerland

Abstract:
At polar discontinuities, i.e. at interfaces between systems with different electric polarization, bound and free carriers appear in order to screen the resulting polarization charges. This mechanism is believed to be the driving force for the emergence of the two-dimensional electron gas at oxide interfaces, giving rise to manifold exciting novel phenomena. Similar processes have also been posited to take place at polar discontinuities between different 2D materials [1,2]. Recently, we have suggested several realistic strategies to engineer such polar discontinuities in 2D materials [3,4], and some are starting to find confirmation in current experiments [5].

Here, we develop further the paradigm and show by first-principles simulations that some 2D polar materials can display a metastable non-polar phase, such that a boundary between the stable and metastable phases supports a polar discontinuity and the resulting 1D metallic wire [6]. We suggest several approaches to realize such phase boundaries by inducing metastable phases in a single parent crystal. Finally, we show how this approach could allow promising opportunities to manipulate and reconfigure 1D electron/hole wires or switch their conduction state.

[1] N.C. Bristowe et al., Phys. Rev. B 88, 161411 (2013).
[2] R. Martinez-Gordillo and M. Pruneda Prog. Surf. Sci. 90, 444 (2015).
[3] M. Gibertini, G. Pizzi, N. Marzari, Nature Commun. 5, 5157 (2014).
[4] M. Gibertini and N. Marzari, Nano Lett. 15, 6229 (2015).
[5] S. Barja et al., Nature Phys. 12, 751 (2016).
[6] M. Gibertini and N. Marzari, in preparation (2016).

Title: **Local density fitting within a Gaussian and plane waves approach to enable large-scale DFT simulations**

Dorothea Golze
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Department of Applied Physics
COMP Centre
Espoo, Helsinki, Finland

Abstract:
A local resolution-of-the-identity (LRI) approach is introduced for Kohn-Sham (KS) density functional theory calculations using a mixed Gaussian and plane waves (GPW) approach within the CP2K program package. The locality of the density fitting ensures that the linear scaling of the GPW approach is retained, while the prefactor for calculating the KS matrix is drastically reduced. In LRIGPW, the atomic pair densities are approximated by an expansion in one center fit functions. Thereby, the computational demands for the grid-based operations become negligible, while they are dominate for GPW.

The LRI approach is assessed for a wide range of molecular and periodic systems yielding highly accurate results for reaction energies as well as intra- and intermolecular structure parameters. Employing LRI, the SCF step is sped up by a factor of 2-25 depending on the symmetry of the simulation cell, the grid cutoff and the system size.

Title: **Electronic and optical properties of Weyl semimetals based on transition metal monopnictides: Ab initio studies of TaAs, TaP, NbAs and NbP**

Davide Grassano
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Rome, Italy

Abstract:

We investigate electronic, optical and loss properties of the topological Weyl semimetals[1] TaAs, TaP, NbAs and NbP[2] crystallizing in bct geometry by means of the ab initio density functional theory with spin-orbit interaction and within the independent-particle approximation. Chemical trends are discussed. The four band structures show well energetically separated Ta5d/Nb4d conduction and As4p/P3p valence bands. Their small band energy overlap leads to electron and/or hole pockets near the Fermi energy ε_f at the 8 W1 and 16 W2 Weyl nodes, the properties of which are computed, in particular for the linear bands and the small energy distances between ε_f and the Weyl nodes. The bands and their occupation near the Weyl nodes determine the infrared optical properties. They give rise to almost constant values of the imaginary part of the dielectric function and, hence, a linear increase of the real part of the optical conductivity. The high-energy spectra are dominated by interband transitions in the band structure. The energy zeros of the real part of the dielectric function define plasmon frequencies, at which the energy loss function exhibits a pronounced peak. The details of the Weyl nodes are compared with recent ARPES results for TaAs and NbP[3-4], and we directly compare with measured optical spectra for TaAs[5].

[1]Weng, Hongming, et al. PRX 5.1(2015):011029
[2]Lee, Chi-Cheng, et al. PRB 92.23(2015):235104
[3]Lv, B. Q., et al. PRX 5.3 (2015): 031013
[4]Souma, S., et al. PRB 93.16(2016):161112
[5]Xu, B., et al. PRB 93.12 (2016): 121110

Title: **Charge-Density-Wave state in TiSe2 single-layers**

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Bellaterra, Cerdanyola del Valles
Barcelona, Spain

Abstract:

In the last years, 2D materials have gotten the attention of many researchers due to their unique properties and tolerance toward manipulation. In this work we focus our attention on the highly debated transition metal dichalcogenide TiSe$_2$ in its monolayer phase. For over a decade the transition from the semi-metallic state to the charge density wave state of TiSe2 has been disputed. Here we discuss, based on density functional theory calculations, how this phase transition is a process mediated by the coupling of electrons with the lattice vibrations. As a consequence of this distortion, the monolayer TiSe2 loses its conductive properties. The retrieval of these properties is also studied and presented here as a function of doping.In the last years, 2D materials have gotten the attention of many researchers due to their unique properties and tolerance toward manipulation. In this work we focus our attention on the highly debated transition metal dichalcogenide TiSe$_2$ in its monolayer phase. For over a decade the transition from the semi-metallic state to the charge density wave state of TiSe2 has been disputed. Here we discuss, based on density functional theory calculations, how this phase transition is a process mediated by the coupling of electrons with the lattice vibrations. As a consequence of this distortion, the monolayer TiSe2 loses its conductive properties. The retrieval of these properties is also studied and presented here as a function of doping.

Title: **Metallic nanoparticles under realistic electrochemical conditions**

Nicolas Hoermann
Theory and Simulation of Materials (THEOS), EPFL
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Abstract:
We present a study of the stability and equilibrium shape of metallic nanoparticles in electrochemical environments based on periodic density functional theory (DFT) calculations.

Metallic surfaces in water are modelled within the self-consistent continuum solvation scheme (SCCS) [2] as recently implemented in the ENVIRON module of Quantum-ESPRESSO [3]. We analyse in detail the effect of the dielectric environment and different adsorbates on surface structure, energetics and potential [4].

The effects of applied potential are treated by studying appropriately charged systems, with explicit countercharge layers in the solution to mimic the effects of the electrical double layer [5]. We will also discuss the difference between this approach and the widely applied ``computational hydrogen electrode''[6] with respect to surface termination and adsorbate species. Our results shed light on how to apply ab-initio thermodynamics in electrochemical environments.

[1] A. Jain et al., APL Materials 1, 011002 (2013)
[2] O. Andreussi, et al., J. Chem. Phys. 136, 064102 (2012).
[3] P. Giannozzi, et al., J. Phys.: Condens. Matter 21, 395502 (2009).
[4] F. Gossenberger, et al., Beilstein J. Nanotechnol. 5, 152 (2014).
[5] N. Bonnet, et al., Phys. Rev. Lett. 110, 086104 (2013).
[6] J. K. Norskov, et al., J. Phys. Chem. B 108, 17886 (2004).

Title: **Computational Methods in Elucidating Mechanisms of Heterogeneous Catalysis**

Matej Huš
National Institute of Chemistry
Department of Catalysis and Chemical Reaction Engineering
Ljubljana, Slovenia

Abstract:
DFT was used to elucidate pathways, intermediates and catalyst structure in reactions over heterogeneous catalysts.

Carbon dioxide valorisation is achieved by hydrogenation to methanol, which is useful as an easy-to-transport fuel or as a raw material in chemical industry. Reaction of CO2 with H2 over CuZn/alumina catalyst is studied using plane-wave DFT. A complex network of all possible reactions between all intermediates is investigated. Reaction rates, equilibrium constants and adsorption are calculated. Among several possible routes, formate route was shown to predominate and formation of H2COO to be the rate-limiting step. Reaction proceeds via EIey-Rideal mechanism.

Lignin is an important component of biomass. Eugenol has been used as a model compound for lignin hydrodeoxygenation. Reaction was carried out in a pressurised reactor over ruthenium catalyst. Two competitive pathways are observed, as first either aromatic ring can be hydrogenated or oxygen-rich substituents can be cleaved off. The end product is always propylcyclohexane. DFT calculations were used to explain the exact mechanism of hydrogeoxygenation and obtain the necessary data to supplement the micro-kinetic model. Reaction proceeds via Langmuir-Hinshelwood mechanism.

Butane is an abundant organic compound with relatively low value. Industrially, it is dehydrogenated to butene and butadiene, with especially the latter having a considerable greater value. NiMoO4 is a widely used catalyst for oxidative dehydrogenation of butane. Instead of oxygen, we used soft oxidants N2O and CO2, which markedly increased selectivity. DFT calculations were used to elucidate the catalyst surface structure and the energetics and kinetics of Mars van Krevelen mechanism.

Title: **Hybrid functional study of P, As, Sb and Bi induced defect levels in Ge**

Emmanuel Igumbor
Samuel Adegboyega University
Ogwa-Edo, Nigeria

Abstract:
The hybrid functional of Heyd, Scuseria, and Ernzerhof (HSE), has been used to calculate the structural and electronic properties as well as the formation and charge state transition energy levels of X (P, As, Sb and Bi) substitutional (X_Ge) and interstitials (I_X) in Ge. While the formation energies of the P, As Sb and Bi substitutions in Ge varied from 0.61 to 1.90 eV, for the interstitial, the formation energies varied from 3.53 to 6.69 eV. The double substitutions in Ge (X_2Ge) is not stable for all X. The charge state transition levels induced by the P, As, Sb and Bi in Ge for both the X_Ge and I_X are not stable within the band gap of Ge. The +2 and neutral charge states are stable for all Fermi energy for the X_Ge and I_X , respectively.

Title: **Thermal conductivity of 2D materials from first principles**

Sergio Illera
Consejo superior de investigaciones cientificas (CSIC) ICMAB
Bellaterra, Spain

Abstract:
From the fundamental science point of view, the heat transport properties are strongly related to the material's structure and composition down to the atomic scale. When the dimensionality is reduced or nanometric scales are reached, novel thermal properties emerge which are not well described using the classical Fourie's law in contrast to their bulk counterpart.

Concerning 2D materials, graphene which is the prototypical 2D material shows exceptional electrical and thermal properties. Experimental thermal conductivity measurements in high quality single-layer graphene samples range between 1500 and 5000 W/(m.K) at room temperature. The exceptional properties of carbon-based honeycomb structures have stimulated strong interest in isomorphic materials, such boron nitride (BN).

We concentrate on the study from first-principles of the thermal transport properties using the methodology of "Approach to Equilibrium Molecular Dynamics". However, this study was carried out using a pure Density Functional Theory (DFT) approach as implemented in the SIESTA program to describe BN instead of the classical force fields. The anisotropy of the thermal conductivity of BN was studied by DFT in combination with MD in order to demonstrate the capabilities of the proposed methodology, and to test the validity of the recent force field studies, quantifying the variation of the thermal conductivity as a function of the transport direction.

This is the first time that both approaches (DFT+AEMD) are used in combination opening the possibility to determine accurately the thermal conductivity in structures which force fields are not available or sufficiently accurate (defective materials, doped systems or surfaces with adsorbates).

Title: **First-principles study of anomalous Nernst effect in skyrmion crystals**

Fumiyuki Ishii
Kanazawa University
Kanazawa,Japan

Abstract:

The magnetic skyrmion, a topological object made up of spins in condensed matter, exhibits many peculiar properties, among which we target the anomalous Nernst effect (ANE), heat-to-electricity conversion in transverse direction, driven by an emergent magnetic field B originating from its spin texture. We have so far found from computations on some models that, in the so-called 2D SkX phase, where skyrmions are crystallized in two dimensions, the crystal-momentum component of B gives rise to the band structure that could generate large ANE when chemical potential μ is properly tuned [1]. Although this behavior was most clearly confirmed in the simplest model of square SkX with single s-orbital per site, our subsequent computations on more realistic models of oxides thin-films also showed possible large ANE. In this presentation, such intriguing results, the details of our first-principles computational procedures, as well as the origin of large ANE will be discussed.

Title: **First principles study of electron scattering mechanism at SiC/SiO2 interface**

Shigeru Iwase
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University of Tsukuba
Tsukuba, Obaraki
Japan

Abstract:
For the development of power electronic devices based on silicon carbide (SiC), one of the main issue is identification and management of killer defects that degrade device performance and reliability. In particular, the attribution of defects to the low carrier mobility at SiC/SiO2 interface is not well characterized and understood. Although extensive experimental characterizations have been performed so far, the relationship between the specific defect and carrier mobility is still unclear and the underlying physics is totally lacking. In this work, we investigate the effect of several C and O related defects on the electron-transport property of 4H-SiC(0001)/SiO2 interface using first-principles calculation. Since there are two types of 4H-SiC(0001) surface depending on the stacking sequence of SiC bilayer, we employ two interface models, which are referred to as h and k type interfaces. We find that the interface type plays a decisive role in electron-transport property rather than species of defects. This is explained by the floating nature of the conduction band edge (CBE) state where wave functions are distributed along the interstitial channels in 4H-SiC. When defects are introduced to the SiC bilayer or between SiC bilayer, they break the interlayer symmetry and may remove the floating state, i.e., CBE state of 4H-SiC. CBE state is started from the first SiC bilayer relative to interface for h type interface, and from second SiC bilayer for k type interface, thus the h type interface is more easily affected by interface defects.

Title: **Lattice matched interfaces between semiconductor alloys and metals**

Line Jelver
Technical University of Denmark
Lyngby, Denmark

Abstract:

Epitaxially matched semiconductor/superconductor interfaces has recently been shown to be a method for creating a material with hard gap induced superconductivity [1] . The two semiconductor alloys InAs 1−x Sb x and Ga x In 1−x As are combined with a selection of metals to make a semiconductor/metal interface. The interface builder in VNL is used to calculate the strain between the two surfaces of the interface and the alloy parameter x, corresponding to zero strain, is found.

Title: **Self-Interaction Effects of Transition Metal Phthalocyanines on Graphene: A DFT Study**

Apichai Jomphoak
Maezono Group
Electronic Structure Calculation Group at JAIST
School of Information Science
Japan Advanced Institute of Science and Technology (JAIST)
Ishikawa, Japan

Abstract:
We present a systematic density functional theory (DFT) study of the electronic structure of selected transition metal phthalocyanines on graphene. In this work, we focuses on copper phthalocyanine (CuPc), nickel phthalocyanine (NiPc), cobalt phthalocyanine (CoPc), and iron phthalocyanine (FePc). Self-consistency simulations for a molecular structure, bond length and angle, formation, stability, adsorption sites, and binding energies of graphene/MPcs composite material are systematically discussed and carried out by employing DFT with LDA/PWC, GGA/PBE, and hybrid exchange-correlation, B3LYP, functionals. Bond lengths and angles obtained with the different functionals utilized in this work are compared to experimental photoemission data. Our results indicate that, among these formations, CoPc has the shortest interplane distances between MPcs and a graphene layer. For HOMO-LUMO gap of graphene/CoPc is much lower than those for graphene or CuPc, NiPc, or FePc. This indicates an enhancement of reactivity in the graphene/CoPc structure, resulting in a potential candidate for a better charge transport and a high quality transparent conductive material.

Title: **Two-dimensional electron gases at head-to-head and tail-to-tail domain walls in ferroelectric thin films**

Francisco Javier Junquera Quintana
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Departamento de Ciencias de la Tierra y Fisica
de la Materia Condensada
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Abstract:

Symmetry breaking at ferroelectric domain walls gives rise to new physical properties, offering the opportunity to use the domain walls themselves as a functional separate object in a device. One example is the appearance of an enhanced conductivity at the boundaries between ferroelectric domains in oxides.

A realistic first-principles simulation of the domains walls is limited to highly symmetric cleanly-cut walls in order to keep the number of atoms in the simulation box small. Here we use a recently developed second-principles method that treats all the lattice degrees of freedom and the relevant electronic ones on the same foot with high accuracy at a modest computational cost. We apply it to the demading physical problem of head-to-head (HH) and tail-to-tail (TT) domain walls in ferroelectric PbTiO$_{3}$ thin films. These interfaces present a large and unfavourable electrostatic energy due to the polarization-induced bound charge at the domain wall. An accurate simulation should capture eventual charge transfers between the walls, and the concomitant electron-lattice coupling. We show how the polarization discontinuity in HH and TT domain walls in PbTiO$_{3}$ thin films can be effectively screened by the formation of two-dimensional electron gases of electrons and holes, respectively.

Finantial support from MINECO Grant No. FIS2012-37549-C05-04

Title: **The pinball model - A frameworkf for the search for solid-state electrolytes**

Leonid Kahle
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Lausanne, Switzerland

Abstract:

Studying and understanding diffusion of ionic charge carriers in solid state is fundamental to the search for new electrolyte materials. Molecular dynamics simulations can be used to gain new insight into diffusion mechanisms and to guide the search for new materials in a high-throughput screening approach. To avoid the need for accurate, but computationally expensive first principles molecular dynamics simulations, we exploit the different behaviour of the host lattice and the diffusing ions, which we simulate as moving in a frozen potential energy landscape derived from the ground state charge density. We compare our model with Born-Oppenheimer molecular dynamics for several Lithium-ion conductors of the thio-LISICON and NASICON family.

Title: **Quantum mechanical simulation of cobalt based magnetic coverages on two dimensional WS2 semiconductor**

Hamideh Kahnouji
Isfahan University Of Technology
Department of Physics
Isfahan, Iran

Abstract:

using density-functional theory, we explore structural stability, electronic and magnetic properties of the 2D heterostructure Co/WS2, consisting of a monolayer of Co atoms desposited on a single WS2 sheet. the spin-polarized DFT calculations were carried out within a general gradient approximation by Perdew, Burke, and Ernzerhof, as implemented in Quantum Espresso package. The effect of van der Waals (vdW) interactions was included for weak interaction cases and described using vdW-DF.we come to the fully covered MoS 2 with Co atoms adsorbing Different positions, such as W-top, S-top and hollow site should be considered. our calculations show that the W-top site is the most stable one. And the hollow and S-top site are 0.68 and 1.09 eV higher in energy, respectively.

Title: **DFT study of fundamental properties of α''-Fe16C2 phase and martensite decomposition at low temperature**

Dmytro Kandaskalov
IM2NP
Marseille, France

Abstract:

Steel is the structural material by far the most used by man, and its role in the global economy is paramount. Some Fe-C phases are of crucial importance in the design of the material properties of steels and ferrous alloys. Among its various forms of Fe-C structures, the martensite is one with highest strength.
The main objective of our work is to address this lack of basic knowledge related to martensite low temperature ageing, most likely by spinodal decomposition toward ferrite (α-Fe wt%C≈0%) and some rich C domains (wt%C≈11%) of unknown structure. Theoretically several structures have been proposed and the most prominent among them is the tetragonal α''-Fe16C2 ordered phase which is isomorph to α''-Fe16N2.
Our theoretical DFT work consist in the study of fundamental properties of α''-Fe16C2 phase as structural, electronic, magnetic, vibrational and elastic properties to better understand the stability of this phase relatively to α''-Fe16N2 . We have shown that this phase is mechanically and dynamically stable. Secondly to elucidate martensite decomposition by spinodal mechanism we have studied some thermodynamic properties of intermediate compounds Fe16Cx (0

Title: **vdW-DF + U description of solid oxygen at low pressure**

Shusuke Kasamatsu
The Institute for Solid State Physics
the University of Tokyo
Chiba, Japan

Abstract:

Oxygen is known to solidify at low temperatures and is very unique in that it becomes a molecular crystal comprised of spin-polarized molecules. However, the description of solid oxygen within the conventional (semi)local density functional approximations used in the Kohn-Sham formalism of density functional theory has been known to be quite unsatisfactory. Recently developed vdW-DF functionals solve the problem partially, but due to inaccurate description of the exchange interaction, the predicted lattice parameters of the ground state antiferromagnetic alpha phase are still off by as large as 15% compared to experiment. The difficulty lies in the subtle balance between the van der Waals interactions and the exchange coupling between the antiferromagnetic and ferromagnetic molecule pairs in the molecular crystal. In this work, we report that the DFT+U approach used in combination with certain vdW-DF functionals performs surprisingly well in this regard [*]. This is explained by the correction of overbinding between antiferromagnetic O2 pairs due to the on-site U interaction applied on the O p orbitals.

[*] S. Kasamatsu, T. Kato, and O. Sugino, arXiv:1606.08568 [cond-mat.mtrl-sci]

Title: **Atomic-scale investigation of grain boundary motion in graphene**

Dongwook Kim
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Seoul, Rep. of Korea

Abstract:
Grain boundaries (GBs) in graphene can migrate when irradiated by electron beams from a transmission electron microscope (TEM). Here, we present an ab initio study on the atomic scale mechanism for the GB motion with misorientation angle of 30° in graphene. From total energy calculations and energy barrier calculations, we find that a Stone--Wales(SW)-type transformation can occur more easily near GBs than in pristine graphene due to a reduced energy barrier. There are other cases of migration which can be understood by other type of transformation, named "evaporation of a carbon dimer". We also find that a mismatch in the crystalline orientation at GBs can drive the evaporation of a carbon dimer easily by greatly reducing the corresponding overall energy barrier. After evaporation of the carbon dimer, the GBs can be stabilized through a series of SW-type transformations that result in GB motion. The GB motion induced by evaporation of the dimer is in excellent agreement with recent TEM experiments.

Ttitle: **Electronic and ionic transport of ions in water confined in carbon nanotubes: a combined first principles calculations**

Alexsandro KIRCH
Universidade de São Paulo
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Abstract:

Nowadays, there is a strong interest on confined fluids at nanoscale for developing devices for nanofluidics applications. For example, through external electric field, it was shown that it is possible to modulate ionic conductivity, promoting nanofluidic systems as a logical transistor. Here, we combine first-principles electronic transport calculations with molecular dynamics (MD) to determine the electronic and ionic transport of ions through an aqueous solution confined at carbon nanotubes (CNT). Using classical molecular dynamics, we have investigated the ions (H, Li, Na and Cl) in aqueous solution flow within (6,6) metallic CNTs. To access the effects of the ions on the CNT electronic transmittances, calculations using non-equilibriums Greens Functions methodology has been performed based on snapshots from MD calculations using the Transampa codes. The results suggest that Li, Cl, Na and H insertion in the Carbon nanotubes lead to different levels of doping. Due to size constrains, the (6,6) CNT allows only the flow of a single line of atoms or molecules, and thus, the ion is not completely solvated. However, even in the presence of water, the influence of these ions on the carbon nanotubes electronic properties has shown to be significant in the Dirac cone displacement. Based on state-of-art first principles calculations, we have been able to characterize the electronic and ionic current of confined fluids (electrolytic aqueous solution) with CNT. In particular, an electronic current signature of distinct ions can been observed, which could lead to potential applications as sensors and nanofluidic devices.

Title: **Ab Initio Statistical Mechanics of Martensitic Phase Transition in NiTi Shape Memory Alloy (SMA)**

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Abstract:

NiTi exhibits a shape memory effect in which it returns to a predetermined shape when heated. The mechanism of this effect is fundamentally related to martensitic transformation, in which NiTi changes from a high temperature cubic (B2) phase to low temperature monoclinic (B19')[1] phase. The transformation is a displacive first order phase transition including change in the crystal shape[2]. Using cubic B2 phase as a reference structure, we develop an effective Hamiltonian to capture its low-energy structural distortions that are relevant to the martensitic phase transitions, and determine all its parameters from first-principles density functional theory calculations. Our model contains the physics of nonlinear elasticity and coupling between strain and phonons. We present statistical mechanical analysis of the effective Hamiltonian using Monte Carlo simulations and establish the martensitic transformation at 260 K from B2 to B19', in good agreement with experimental transition temperature of 310 K. We uncover the specific coupling and mechanism that govern the B2 to B19' structural phase transitions.

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Title: **First-principles studies of valence band structure, core level binding energy, and phonon dispersion of epitaxial silicene on zirconium diboride (0001) surface**

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Abstract:

Silicene has caught great attention recently. An important issue is to demonstrate the successful fabrication of silicene by experiments beyond just a theoretical proposal. Within the framework of density functional theory, we have studied silicene on the zirconium diboride (0001) surface[1,2] and found that the valence band structure,[3] core level binding energy,[4] and phonon dispersion[5] are all in good agreement with experiments, providing solid supports of the existence of planar-like silicene on the zirconium diboride (0001) surface. Specifically, we have unfolded the band structure to a one-atom zone where only the states possessing long lifetime can show large spectral weight, allowing easy comparison with the angle-resolved photoelectron spectroscopy. In studying core level binding energy, we have implemented an exact Coulomb-cut off technique, allowing direct access of many-body total energies of (N)- and (N-1)-electron systems.[4,6] The phonon study has revealed the mechanism of appearance of large-scale stripe patterns, which is consistent with the scanning tunneling microscope images.[1,5] Our study also indicates that density functional theory is successful in describing the many-body total energy, the forces between atoms, and the electronic band structure of valence electrons for the case of silicene on the zirconium diboride (0001) surface.

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Title: **Microfaceting of Cu$_2$O and its implications in photochemistry**

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Abstract

The high Miller-index microfacets e.g. \{211\}, \{311\}, and \{522\} have been proposed to play a key role in shape-controlled crystal engineering of Cu$_2$O polyhedrons for various clean energy applications [1]. These Cu$_2$O microcrystals with high Miller-index microfacets are found to have a higher photocatalytic activity than those with octahedra and cube morphologies, and thus suggesting that the catalytically active sites are more abundant on the high Miller-index surfaces. Although much effort has been devoted to the actual synthesis and characterizations of these shaped Cu$_2$O nanocrystals with various morphologies, a firm theoretical understanding of these system are currently limited to low Miller-index facets of Cu$_2$O [2]. Here, we perform first-principles density-functional theory (DFT) calculations using the Vienna {\it ab initio} Simulation Package (VASP) to study the surface energetics and electronic structure of these high Miller-index Cu$_2$O surfaces, and evaluate their overpotential for water redox reactions on Cu$_2$O, in comparison with that for the low Miller-index surfaces.

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Title: **Enhanced magnetoelectric coupling in multiferroics from atomistic simulations**

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Abstract:
Multiferroics have attracted an unprecedented attention in the recent years owing to their potential to exhibit magnetoelectric coupling. Such coupling could open the ways to innovative applications such as four-state logic in a single device, magnetoelectric random access memories, electrically controlled exchange bias applications. Most of these applications, however, require strong coupling between electric and magnetic degrees of freedom. We propose an unusual route to a robust enhancement of magnetoelectric coupling via thermally mediated mechanism. Such mechanism couples magnetization to the electric field (polarization to the magnetic induction) indirectly by taking advantage of pyromagnetic and electrocaloric (pyroelectric and magnetocaloric) properties of the material. This approach was tested in both direct and indirect first-principles-based simulations of multiferroic $BiFeO_3$.

Title: **Modeling Thiolate-Gold interface for protected nanoparticles**

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Abstract:

Self-assembled monolayers (SAMs) are aplied to gold nanoparticles to guide growth, increase stability, and provide additional functionality. However, as with any surface coating, the changes to the energetics of the surface can have unanticipated consecuences, as well as introducing new oportunities. Understanding the relationship between the coverage degree and type of the SAMs and the underlaying gold nanoparticles is challenging, but can be explored very efficientely using modeling and computational simulations. In that sense, very recently we have developed a semi-empirical many-body potential, fitted from DFT calculations, wich takes account many differents abossortions sites for MethilThiolate on Gold Surfaces.

Title: **Indiene - a new monolayer material**

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Abstract:

One atom thick monolayer nanostructures consisting of group III, IV and V elements are drawing ever more attention for their extraordinary electronic properties. Through first principles calculations, we systematically investigate structural and electronic properties of the corresponding indium monolayers in three different allotropic forms: planar, puckered and buckled. Our study shows that the planar and buckled allotropes are stable and show metallic and semiconducting behavior, respectively. Their stability and electronic properties cannot be easily correlated to those of similar elemental monolayer structures. The van Hove singularity is observed in the electronic density of states which could lead to an increase in the electronic conductivity, opening paths to new electronic applications. Strain engineering is applied in order to determine the changes in the electronic behavior and band gap properties. The planar allotrope remains metallic under both compressive and tensile strain, while the buckled allotrope changes from an indirect semiconductor to a metal. Our study demonstrates that the indiene nanostructures possess diverse electronic properties, tunable by strain engineering, which have potential applications in nanoelectronics and for nanodevices.