Title: **Electronic properties of BN-doped T graphene: A density functional theory study**

Roya Majidi
Department of Physics
Shahid Rajaee Teacher Training University
Tehran, Iran

Abstract:

We have studied the effect of impurity on the electronic properties of T graphene. The electronic band structures and density of states were calculated based on density functional theory as implemented in the OpenMX3.6 package. It was found that T graphene was a metal. The impurity has a considerable effect on the electronic properties of T graphene. The B-doped and N-doped T graphene were become p-type and n-type semiconductors, respectively.

Title: **Electronic and optical properties of hexathiapentacene in the gas and crystal phases**

Giuliano Malloci
Dipartimento di Fisica
Università degli Studi di Cagliari
Monserrato, Italy

Abstract:
Using DFT and its TD extension, the electronic and optical properties of the hexathiapentacene (HTP) molecule, a derivative of pentacene (PNT) obtained by symmetric substitution of the six central H atoms with S atoms, are investigated for its gas and solid phases. For the molecular structure, all-electron calculations are performed using a Gaussian localized orbital basis set in conjunction with the Becke three-parameter Lee-Yang-Parr (B3LYP) hybrid exchange-correlation functional. Electron affinities, ionization energies, quasiparticle energy gaps, optical absorption spectra, and exciton binding energies are calculated and compared with the corresponding results for PNT, as well as with the available experimental data. The DFT and TDDFT results are also validated by performing many-body perturbation theory calculations within the GW and Bethe-Salpeter equation formalisms. The functionalization with S atoms induces an increase of both ionization energies and electron affinities, a sizable reduction of the fundamental electronic gap, and a redshift of the optical absorption onset. Notably, the intensity of the first absorption peak of HTP falling in the visible region is found to be nearly tripled with respect to the pure PNT molecule. For the crystal structures, pseudopotential calculations are adopted using a plane-wave basis set together with the Perdew-Burke-Ernzerhof exchange-correlation functional empirically corrected in order to take dispersive interactions into account. The electronic excitations are also obtained within a perturbative B3LYP scheme. A comparative analysis is carried out between the ground-state and excited-state properties of crystalline HTP and PNT linking to the findings obtained for the isolated molecules.

Title: **High-throughput search for Z2 topological insulators in two dimensions**

co-Authors: **Antimo Marrazzo *), Marco Gibertini, Nicolas Mounet, Davide Campi and Nicola Marzari**

* Theory and Simulation of Materials (THEOS),
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Lausanne, Switzerland

Abstract:
Topological materials are a novel class of solids with outstanding properties protected by an interplay of topology and symmetry. Some of the hosted phenomena---such as dissipationless electron transport or spin filtering---are very promising for technological applications in many fields like electronics and spintronics. The rarity of known materials exhibiting a stable topologically non trivial phase at room temperature---especially in two dimensions---has hindered their technological applications so far. In this work we screen a database of exfoliable 2D materials, by explicitly computing the Z2 topological invariant from first principles at the level of DFT-PBE with spin-orbit coupling. A refinement at the G0W0@PBE level is also done for the interesting candidates. This enables us not only to search for novel 2D topological insulators, but also to estimate the abundance of these materials in two dimensions.

Title: **Electronic and magnetic properties of zigzag graphene nanoribbons deposited on the topological insulator Sb2Te3**

Riccardo Mazzarello
RWTH Aachen
Institute for Theoretical Solid State Physics
Aachen, Germany

Abstract:

Zigzag graphene nanoribbons (GNRs) are predicted to possess spin-polarized electronic states confined at the edge, with antiferromagnetic coupling between the two edges. However, the robustness of this phenomenon is under debate. In this work, we present a density functional theory investigation of zigzag GNRs deposited on the (111) surface of the topological insulator Sb2Te3. The strong spin-orbit coupling induced by this substrate could stabilize edge magnetism against quantum and thermal fluctuations. Moreover, it is interesting to assess the possible back action of edge magnetism on the surface state of Sb2Te3. We show that, for H-terminated GNRs, the interaction between the GNR and the substrate is very weak. As a result, the surface-GNR distance is large and the magnetic anisotropy energy induced by substrate is small. On the other hand, the strong chemical interaction between the H-free GNR and the topmost Te layer of Sb2Te3(111) leads to the bending of the GNR and a chiral magnetic configuration stabilized by the interplay between the inter-edge exchange interaction, the magnetic anisotropy energy and the Dzyaloshinskii-Moriya interaction. This magnetic configuration induces a small shift of the Dirac point of the surface state.

Title: **Accelerating ab-initio Molecular Dynamics and probing the weak dispersive forces in dense liquid hydrogen**

Guglielmo Mazzola
ETH Zurich, Switzerland

Abstract:
We propose a new ab-initio molecular dynamics method, capable to reduce dramatically the auto- correlation time required for the simulation of classical and quantum particles at finite temperature. The method is based on an efficient implementation of a first order Langevin dynamics modified by means of a suitable, position dependent acceleration matrix. Here we apply this technique both on a Lennard-Jones toy model and within a Quantum Monte Carlo (QMC) based wavefunction approach, for determining the phase diagram of high-pressure Hydrogen. With the proposed method, we are able to equilibrate in few hundreds steps even close to the liquid-liquid phase transition (LLT). We find that the LLT transition is consistent with recent density functionals predicting a much larger transition pressures when the long range dispersive forces are taken into account.

Title: **A first principles view of nanoaggregation of asphaltenes and their adsorption processes on carbonate surfaces**

Caetano Miranda
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Institute of Physics
Department of Mechanics and Materials Physics
São Paulo, Brazil

Abstract:
Asphaltenes are large organic molecules found in crude oil and have the ability to aggregate and adsorb on the surface of natural reservoirs. Their aggregation and absortion properties can affect the whole oil supply chain production. The adsorption mechanisms of these molecules on the minerals surfaces can be the basis for understanding a proper chemical mechanism for the nanoaggregation of asphaltene and resins molecules, particularly for carbonate reservoirs. However, so far, the interaction mechanisms between these organic molecules and the surface of calcite (CaCO3) are unknown. These systems impose a challenging description at electronic level that is required to understand the process phenomenology. Using first-principles calculations based on density-functional theory (DFT) with van der Waals (vdW) dispersion, we studied the nanoaggregation and adsorption of asphaltene, resin, and resin–asphaltene aggregates on the calcite (10.4) surface in the presence of a dielectric water–toluene environment. A nanoaggregation mechanism is proposed based on the competition of the pi-orbitals, leading to a degeneracy of the electronic states. The heteroatoms´ role is important to influence the charge rearrangement, increasing thus the interaction among the aliphatic chains and aromatic groups. Our calculations also indicate that there is a minor steric hindrance in the effective interaction of the aromatic region of asphaltene on the calcite surface. These findings shed light on important adsorption mechanisms and aggregation processes of organic nanoaggregates in surfaces and it can guide new methods for asphaltene stability control. In collaboration with R. S. Alvim and F.C. D. A. Lima under Petrobras grant.

Title: **Dimensionality effects on magnetic properties of FexCo1-x nanoclusters on Pt(111): an ab initio investigation**

Ivan Miranda
University of São Paulo
Department of Mechanics and Materials Physics (DFMT)
São Paulo, Brazil

Abstract:
The search of new magnetic materials has been attracting large interest in the last decades, notably due to their unconventional behaviors and spin structures observed at the nanoscale. These behaviors can arise from the combination of spin-orbit coupling with broken inversion symmetry, related, for instance, to the reduced dimensionality. In this context, FexCo1-x nanoclusters deposited on the Pt(111) surface are investigated with the RS-LMTO-ASA method in the framework of the DFT. Different configurations of triangular trimers and hexagonal heptamers are considered, varying the positions and concentration of Fe/Co atoms. We demonstrate the occurrence of a strictly decreasing nonlinear trend of the average orbital moments with the Fe concentration for the compact clusters, distinct from what was found not only for FexCo1-x/Pt(111) nanowires, but also for higher-dimensional systems (monolayer and bulk). In turn, the collinear average spin moments are described by a linear function with respect to stoichiometry. In all studied cases, the nearest neighbors exchange interactions have shown to be strongly ferromagnetic, although their values oscillate in further distances. Also, a non-negligible Dzyaloshinskii-Moriya interaction, induced by Pt spin-orbit coupling, is observed for some particular Fe-Co nanoclusters. Among them, we can mention the triangular pure Co trimer and the linear pure Fe heptamer, for which it is obtained a spin density wave.

Title: **First Principle study of CO2 adsorption on TiO2 surface with and without a Graphene Overlayer**

Shashi Mishra
(Dr. Ranjit Kumar Nanda, Associate Professor)
Condensed Matter Theory and Computational Laboratory
Department of Physics,
Indian Institute of Technology Madras, IIT
Chennai. India

Abstract:

Photocatalytic conversion of CO2 is currently being widely studied on TiO2 surface, due to its well-known application in water splitting. However, it is limited due to its relatively large band gap and occurrence of fast electron-hole recombination. Recently, TiO2 surface interfaced with graphene has been proposed as a potential candidate for enhanced visible light absorbance and electron-hole pair separation. In this work, we study using first principles the interaction between CO2 and TiO2 with and without graphene. We have specifically chosen the planar anatase TiO2 (001) as our model surface. CO2 was adsorbed in different orientations on an O site. The ground state structures of the bare and CO2 adsorbed surfaces and the relative stabilities of the latter have been studied.In the future, we plan to investigate the surface dynamics and reactivity towards the adsorbant molecules using ab initio Molecular dynamics. we will also calculate the band gap of the two surfaces and examine the alignment of the band edge positions with respect to the redox potentials. The role of water on TiO2 surface for CO2 conversion will be studied in depth.

Title: **Large-scale first-principles study of Si/Ge core-shell nanowires using a linear-scaling technique.**

Tsuyoshi Miyazaki
International Center for Materials Nanoarchitectonics (MANA)
National Institute for Materials Science
Tsukuba, Japan

Abstract:

I will report the implementation of first-principles molecular dynamics (FPMD) to our linear-scaling DFT code CONQUEST and its application on Si/Ge core-shell nanowires.

In the first part, I will show that efficient and robust O(N) FPMD simulations are now possible by the combination of the extended Lagrangian Born-Oppenheimer molecular dynamics method, which was recently proposed by Niklasson et al., and the density matrix minimization method as an O(N) technique. Since CONQUEST has almost ideal parallel efficiency even when we use more than 200,000 cores, we can conclude that FPMD simulations on million-atom systems are now possible.

In the second part, I will present our recent study on Si/Ge core-shell nanowires (NWs). Si/Ge or Ge/Si core-shell nanowires (NWs) have many attractive properties for next generation devices. We have performed structure relaxation of the core-shell NWs and calculated the structural and electronic properties of different structural models having the actual size of NWs. The analysis of the distribution of the strains of Si/Ge or Ge/Si core-shell nanowires with various sizes and models will be presented. I will also show the Kohn-Sham eigenstates near the Fermi level, which are calculated by applying Sakurai-Sugiura method to the SCF Hamiltonian obtained by O(N) DFT calculations.
This work is done with J. Lin, D. R. Bowler and other CONQUEST members at NIMS and UCL. We also have the collaborations with the experimental group headed by Dr. N. Fukata at NIMS-MANA, and Dr. Y. Futamura and Prof. T. Sakurai at University of Tsukuba.

Title: **The electronic structure of water from Koopmans-compliant functionals**

James Moraes de Almeida
THEOS Theory and Simulations of Materials
Ecole Polytechnique Federale de Lausanne
Lausanne, Switzerland

Abstract:
In this work, we employ a Koopmans-compliant functional [1] (namely, KI [2]) to determine the electronic structure and the band gap of liquid water at room temperature and pressure. First, we provide extensive, equilibrated trajectories for water at normal conditions using a variety of techniques (14 in total) that include classical or first-principles molecular dynamics and/or nuclear quantum effects. For each of these trajectory, twenty uncorrelated samples are chosen and the electronic structure and band gap are calculated at the KI level. We compere these results with experiments, and, where available, with G0W0 calculations. We find that, for the same underlying potential energy surface or molecular dynamics technique, the KI functional delivers results that are essentially equivalent to G0W0, and that might seem even in slightly closer agreement with experiments, but at a fraction of the computational cost. Most notably, different potential energy surface still lead to different results, with a spread of several tenths of an eV when compared with experimental data – we track these discrepancies to the different strengths of the O-H bond in the isolated molecule for the underlying potentials.

[1] I. Dabo, M. Cococcioni, N. Marzari, arXiv:0901.2637 [cond-mat.mtrl-sci] (2009); I. Dabo, et al., Phys. Rev. B 82, 115121 (2010)
[2] Giovanni Borghi, Andrea Ferretti, Ngoc Linh Nguyen, Ismaila Dabo, and Nicola Marzari, Physical Review B, 90, 075135 (2014)

Ttitle: **Computational exfoliation of all known 3D materials**

Nicolas Mounet
Ecole Polytechnique Federale the Lausanne
Institute of Materials, School of Engineering
Theory and Simulation of Materials
Lausanne, Switzerland

Abstract:
As a first step towards the identification of novel and promising 2D materials, we provide here a large scale first-principles exploration and characterization of such compounds. From a combination of 480,000 non-unique structures harvested from the ICSD [1] and COD [2] databases, three-dimensional crystals are screened systematically by checking the absence of chemical bonds between adjacent layers, identifying close to 6,000 layered systems. Then DFT calculations of the van der Waals interlayer bonding are performed with automatic workflows, after full atomic and cell relaxations. In total, more than 1000 two-dimensional structures are found from this screening and are then classified in prototypes according to their similarity. Finally, the metallic, insulating or magnetic character of the materials obtained is assessed systematically. Thanks to the AiiDA materials' informatics platform [3], and in particular its automatic workflow engine, database structure, sharing capabilities, and pipelines to/from crystallographic repositories, the systematic and reproducible calculation of these properties becomes straightforward, together with seamless accessibility and sharing.

[1] http://www.fizkarlsruhe.com/icsd.htm
[2] S. Grazulis et al, Nucleic Acids Research, 40, D420 (2012).
[3] G. Pizzi, A. Cepellotti, R. Sabatini, N. Marzari and B. Kozinsky, Comp. Mat. Sci. 111, 218 (2016).

Title: **Defect Induced magnetization in Graphene**

Ebrahim Nadimi
K. N. Toosi University of Technology
Tehran, Iran

Abstract:
The 2D form of carbon, graphene, has been evolved as a major candidate for post Si era in nanoelectronics. Graphene nanoribbons are serious candidates to be sued in the active channel of future field effect transistors. Although the defects are always a disturbing perturbation in the function of a device the carbon vacancies in graphene, which generally induced by high energetic processes, show interesting magnetic properties. There are interesting works applying ab initio first principles method to investigate the magnetic properties of single carbon vacancy in graphene. However, the formation energy of such defects, the convergence of the calculations and the multiple defects or clustering probability of single defects are not fully investigated. In the present work we present the calculations in the framework of total energy density functional theory to investigate the defect formation energies in fully converged calculations. We find the required supercell size for a converged defect formation energy and calculate the deformations around a vacancy or vacancy cluster to show that using small supercells lead to the overestimation of formation energies. The defect formation energies for double and triple vacancies are investigated for different configurations and a possible clustering of single vacancies are discussed. Based on converged defect geometries we calculate the induced magnetic moment corresponding to each defect or defect complex. The results show that defected graphene could be a promising substrate for spintronic devices.

Title: **Including the effects of atomic bonding in TEM and STEM image simulations**

Timothy Naginey
Materials Modelling Laboratory,
Department of Materials
University of Oxford
Oxford, United Kingdom

Abstract:
Most of the software used to simulate TEM/STEM images completely neglects interatomic interactions in the sample and thus leaves out the effects of charge transfer and chemical bonding. The effect of these interactions on the image is generally small compared to the total charge density, but essential to understanding many important properties of materials. These interactions are especially important for fully quantitative interpretations of TEM/STEM images of certain sample types such as bulk oxides because of the strong ionic bonds, and 2D materials composed of light elements since most of the electrons are involved in bonding. In order to accurately simulate TEM/STEM phase images of these and other such materials, we have employed the CASTEP code to generate accurate projected potentials which take into account both intra- and interatomic electron interactions. CASTEP uses DFT to calculate electron densities, which are directly related to the electrostatic potential via Poisson's equation. These potentials are then used to calculate the projected potentials for use in multislice algorithms to simulate TEM/STEM images. We have added to the functionality of CASTEP so that these projected potentials can be obtained directly from the software, thus allowing us easy and accurate simulation of images with bonding effects included which enables accurate interpretation of experimental images of materials, such as h-BN.

Title: **How does hydrogen peroxide dissociate on Pd-M (M= Cu, Pt) alloy clusters?**

Masoud Nahali
Babol University of Technology
Babol, Iran

Abstract:
Determination of the conditions under which H_2O_2 adsorbs or dissociates on small clusters may help to comprehend the same reactions on nanoparticles which have been used as catalyst in some fuel cells recently. In this work, we have studied H_2O_2 adsorption and spontaneous dissociation on Pd and Pd-alloy small clusters by density functional theory. The hybridisation of the bond orbitals has been calculated to find the orbitals involved in the dissociative adsorption of hydrogen peroxide.

Title: **Optimized multi-site local orbitals in the large-scale DFT code CONQUEST**

Ayako Nakata
First-principles Simulation Group
Nano-Theory Field
International Center for Materials Nanoarchitectonics (MANA)
National Institute for Materials Scienc
Tsukuba, Japan

Abstract:
CONQUEST is a linear-scaling (O(N)) DFT code developed jointly by UCL and NIMS. CONQUEST achieves O(N) by using the locality of density matrices with the density matrix minimization method. Local orbitals which are called support functions are used to express the density matrices and Kohn-Sham orbitals. Our recent study shows that the code can employ DFT calculations on million-atom systems.

We have introduced multi-site support functions [Phys. Chem. Chem. Phys. 17, 31427 (2015)], which are the linear combinations of pseudo-atomic orbitals from a target atom and its neighbor atoms. Multi-site support functions correspond to local molecular orbitals so that the number of required support functions can be the minimal. The linear-combination coefficients are optimized numerically while the initial coefficients are determined by using the localized filter diagonalization method [Phys. Rev. B 80, 205104 (2009)]. The accuracy and computational efficiency of the present method are demonstrated by investigating the atomic and electronic properties of hydrated DNA systems containing several thousand atoms. The test calculations of metallic nanoparticles show the applicability of the method to metallic systems. Since the accuracy of the unoccupied states is not guaranteed in the present method, we have also employed an efficient projection method to obtain the eigenstates in specific energy ranges [J. Comp. Appl. Math., 159, 119 (2003)]. The unoccupied states can be improved by representing the Hamiltonian in primitive basis functions with the optimized density and being recalculated by the projection method.

Title: **Electronic and optical properties of 2D/3D heterojunctions**

Mahesh Neupane
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Aberdeen Proving Ground
USA

Abstract:
With the advent of novel 2D materials such as graphene and TMDC, there have been an increased interest in integrating these 2D materials with their 3D (bulk-like) counterparts for realistic optical and electronic applications. In this study, we highlight some of the theoretical and experimental challenges in studying 2D/3D heterojuctions. As part of the theoretical study, a need for a large scale atomistic approach in modeling realistic heterojunctions is presented, and initial electronic and optical results from the adapted method is compared against our experimental findings.

Title: **Excitons and optical spectra of phosphorene nanoribbons**

Zahra Nourbakhsh
Institute for Research in Fundamental Science IPM
Tehran, Iran

Abstract:
On the basis of many-body ab-initio calculations, using the single-shot G 0 W 0 method and Bethe-Salpeter equation, we study phosphorene nanoribbons (PNRs) in the two typical zigzag and armchair directions. The electronic structure, optical absorption, electron-hole (exciton) binding energy, exciton exchange splitting, and exciton wave functions are calculated for different sizes of PNRs. The typically strong splitting between singlet and triplet excitonic states make PNRs favorable systems for optoelectronic applications. Quantum confinement occurs in both kinds of PNRs, and it is stronger in the zPNRs, which behave like quasi-zero-dimensional systems. Scaling laws are investigated for the size-dependent behaviors of PNRs. The first bright excitonic state in PNRs is explored in detail.

Title: **Density functional based study of boronitrene and its derivatives**

**KO Obodo (1, JT Obodo (2, RC Andrew (3,
N Chetty (3, U Schwingenschlögl (4**

1. University of South Africa
2. University of Nigeria Nsukka
3.University of Pretoria South Africa
4. King Abdullah University of Science and Technology Saudi Arabia

Abstract:

We perform first principles density functional calculations to study the stability, structural and electronic properties of boronitrene and its derivatives. Subsequently, we modify the band offset in a single layer of boronitrene by substituting a single/double line of carbon atoms. This effectively introduces a line of dipoles at the interface. Various junctions of this system with different orientations are considered. The "zigzag-short" structure is found to be the most energetically stable orientation, with formation energy of 0.502 eV and with a band offset of 1.51 eV. We show that specific defect configurations even can result in metallicity, raising interest in the material for electronic applications. We thus study the transport properties of C-functionalized boronitrene using the non-equilibrium Green's function formalism. We investigate various zigzag and armchair defect configurations, spanning wide band gap semiconducting to metallic states. Unusual I–V characteristics are found and explained in terms of the energy and bias-dependent transmission coefficient and wavefunction. In particular, we demonstrate negative differential conductance with high peak-to-valley ratios, depending on the details of the substitutional doping, and identify the finite bias effects that are responsible for this behaviour. The applications of this Nano - based material are mainly in advanced solid-state devices.

Title: **Simple Screened Hydrogen Model of Excitons in Two-Dimensional Materials**

Thomas Olsen
Department of Physics
Technical University of Denmark
Kgs Lyngby, Denmark

Abstract

We present a generalized hydrogen model for the binding energies (E) and radii of excitons in two- dimensional (2D) materials that sheds light on the fundamental differences between excitons in two and three dimensions. In contrast to the well-known hydrogen model of three-dimensional (3D) excitons, the description of 2D excitons is complicated by the fact that the screening cannot be assumed to be local.We show that one can consistently define an effective 2D dielectric constant by averaging the screening over the extend of the exciton. For an ideal 2D semiconductor this leads to a simple expression for E that only depends on the excitonic mass and the 2D polarizability α. The model is shown to produce accurate results for 51 transition metal dichalcogenides. Remarkably, over a wide range of polarizabilities the binding energy becomes independent of the mass and we obtain $E \approx 3/(4\pi\alpha)$, which explains the recently observed linear scaling of exciton binding energies with band gap. It is also shown that the model accurately reproduces the nonhydrogenic Rydberg series in WS2 and can account for screening from the environment.

Title: **Core level binding energies in solids from first-principles**

Taisuke Ozaki
Core level binding energies in solids from first-principles
Institute for Solid State Physics (ISSP), The University of Tokyo
Kashiwa, Japan

Abstract:
A general method is presented to calculate absolute binding energies of core levels in metals and insulators, based on a penalty functional and an exact Coulomb cutoff method in a framework of the density functional theory [1]. The spurious interaction of core holes between supercells is avoided by the exact Coulomb cutoff method, while the variational penalty functional enables us to treat multiple splittings due to chemical shift, spin-orbit coupling, and exchange interaction on equal footing, both of which are not accessible by previous methods. It is demonstrated that the absolute binding energies of core levels for both metals and insulators are calculated by the proposed method in a mean absolute (relative) error of 0.4 eV (0.16 %) for eight cases compared to experimental values measured with X-ray photoemission spectroscopy within a generalized gradient approximation to the exchange-correlation functional.

[1] T. Ozaki and C.-C. Lee, arxiv:1607.05544 (2016).

Title: **Lattice dynamics and thermophysical properties of some h.c.p. elements from the quasi-harmonic approximation**

Mauro Palumbo
Scuola Internazionale Superiore di Studi Avanzati (SISSA)
Trieste, Italy

Abstract:
In this work, we report first-principles lattice-dynamical and anharmonic temperature-dependent properties of several h.c.p. elements calculated using the quasi-harmonic approximation. The evaluated properties range from phonon frequencies to elastic constants and thermodynamic quantities. We compare two approaches for the calculation of the anisotropic thermal expansion tensor: minimizing the Helmholtz free energy and using the Gruneisen parameters. The anisotropic elastic tensor is computed as a function of temperature in the so-called quasi-static approximation. We also compare results obtained by fully evaluating the anisotropic properties of the hexagonal cells and by assuming an isotropic-like behavior, i.e. considering the c/a ratio constant. The results are systematically compared with the available experimental data.

Title: **Improvements on non-equilibrium and transport Green function techniques: the next-generation transiesta**

Nick Papior
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Bellaterra, Barcelona
Spain

Abstract:

We present novel methods implemented within the non-equilibrium Green function code (NEGF) tran-siesta based on density functional theory (DFT).
Our flexible, next-generation DFT-NEGF code handles devices with one or multiple electrodes (N e peratures. ≥ 1) with individual chemical potentials and electronic tem-
We describe its novel methods for electrostatic gating, contour optimizations, and assertion of charge conservation, as well as the newly implemented algorithms for optimized and scalable matrix inversion, performance-critical pivoting, and hybrid parallelization.
Additionally, a generic NEGF post-processing code (tbtrans / phtrans) for electron and phonon transport is presented with several novelties such as Hamiltonian interpolations, N e ≥ 1 electrode capability, bond-currents, generalized interface for user-defined tight-binding transport, transmission projection using eigenstates of a projected Hamiltonian, and fast inversion algorithms for large-scale simulations easily exceeding 10 6 atoms in tight-binding matrices on workstation computers. The new features of both codes are demonstrated and bench-marked for relevant test systems.

Title: **A DFT study of band gap of few layers phosphorene applying in-plane strains**

Mansoureh Pashangpour
Islamic Azad University - Islamshahr Branch
Science Department
Tehran, Iran

Abstract:
We have investigated tuning band gap of mono-, bi- and three layers of phosphorene with applying uniaxial and biaxial strains using first principle calculations based on density functional theory. The results show mono-, bi- and three layers of phosphorene are narrow direct semiconductors with 0.75, 0.45 and 0.23 eV energy gap, respectively and in-plane strains significantly change their bandstructures. Direct-indirect semiconductor and semiconductor-metal transitions induce with uniaxial strains, symmetric and antisymmetric biaxial strains. Dispersion relation at low energy has a linear spectrum shape, Dirac-shaped dispersion, in the metal zone for uniaxial strain along armchair and zigzag directions and for the symmetric strain. Consequently, applying a reasonable strain one can be able controls the size of energy gap and electronic properties of few layers of phosphorene.

Title: **Periodic lattice distortion and electronic structure of monolayer rhenium disulphide ReS2**

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EPFL - School of Basic Sciences
Institute of Physics
Chairs of computational condensed matter physics
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Abstract:

Monolayer rhenium disulphide in the 1T phase (1T-ReS2) is subject to a large periodic lattice distortion resulting in the formation of diamond chains of rhenium atoms associated with a significant shortening of the Re-Re bond length. We show that this distortion is reminiscent of the charge density wave phase observed in many other transition metal dichalcogenides, but is driven by a strong coupling beteween the electron and ions rather than by a simple Fermi surface instability. The effect of the distortion on the electronic bands is large and leads to insulating behavior. The calculated electronic structure exhibits a conduction band that is both narrow and isolated from the other bands, making it sensitive to disorder. Together with transport simulations, we use these results to interpret experimental transport measurements on samples doped with electrolyte ionic gating, where a complete depletion of the conductivity was observed as a result of Anderson localization [1].

[1] D. Ovchinnikov, F. Gargiulo, A. Allain, D. J. Pasquier, D. Dumcenco, C.-H. Ho, O. V. Yazyev and A. Kis, Nature Commun. 7, 12391 (2016).

Title: **Electronic Structure Evolution during the Growth of Graphene Nanoribbons on Au(110)**

Claudia Maria Pereira Cardoso
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Modena, Italy

Abstract:

Molecular monomers with defined size, shape, and chemical functionality are promising and versatile building blocks to produce nanostructured systems with atomic precision through a bottom-up approach. Recently, this approach has been exploited to build up graphene nanostructures. Among these, graphene nanoribbons (GNRs) are on the spotlight of the current research due to their semiconducting properties and promising applications, ranging from spintronics to nano- and optoelectronics. One of the most used molecular precursors to achieve subnanometer-wide GNRs is 10,10′- dibromo-9,9′bianthracene (DBBA). Here we report on a study on the formation of GNRs on Au(110), as based on the surface mediated reaction of DBBA. The formation of GNRs was investigated by means of first-principles calculations within Density Functional Theory at the LDA level. The results complemented the experimental characterization by means of STM, XPS/UPS, NEXAFS. We have studied the molecule/surface interaction at different stages of the GNR formation on Au(110) surface and the evolution of molecular states from monomer DBBA precursors to polyanthryl (PA), and to GNRs. Our results show that initial stages of the reaction crucially determine the final configuration and orientation of the GNRs. We are also able to identify a spectral fingerprint of C−Au interaction in both DBBA single-layer and polymerized chains obtained upon heating and the stronger GNR-Au interaction when compared with PA-Au.

Title: **ENHANCEMENT OF ELECTRON-PHONON COUPLING IN ALKALI-DOPED GRAPHENE AND THIN MgB2 LAYERS**

Jelena Pešić, Igor Popov, Vladimir Damljanović, Radoš Gajić
Graphene Laboratory
Center for Solid State Physics and New Materials
Institute of Physics
University of Belgrade
Belgrade, Serbia

Abstract:
We present first principle investigation of enhancement of the electron-phonon coupling of superconducting alkali-doped graphene (e.g. LiC6-mono) and thin layers of MgB2 using density functional theory (DFT). These systems resemble in many ways, not only in geometry but as well as in electronic structure. Namely, like in alkali-C6, where we have carbon hexagons with alkali adatom in the hollow site, in MgB2 there are boron hexagons with Mg in hollow site. For instance, both theoretical and experimental studies of LiC6-mono proved a possibility of superconductivity in doped graphene. Continuing this investigation, we explored an enhancement of electron-phonon coupling and the raise of critical temperature in LiC6-mono.

Inspired by similarity of intercalated graphite with MgB2, we studied the electron-phonon coupling in MgB2 thin films. We used ab-initio calculations of phonon dispersion and electron-phonon-coupling within framework of DFT using Quantum Espresso. Our research included dopant and strain effects on an enhancement of electron-phonon coupling. We demonstrated an increase of electron-phonon coupling and critical temperatures.

Title: **The effect of strain on Ag+ cation substitution in CdSe nanocrystals**

Urko Petralanda
Italian Institute of Technology
Genoa, Italy

Abstract:

Cation exchange (CE) reactions allow for the selective replacement of the cations of preformed ionic nanocrystals (NC) with new desired guest cations, while retaining their size, shape and anion framework. CE is lacking a full theoretical understanding despite the vast amount of research it has been object of since last decade [1,2].

In a prototypical case, incoming Ag+ cations can rapidly substitute Cd2+ cations in a CdSe NC[3]. In a general view, the incoming Ag+ cations diffuse into the NC from a solvent and, after reaching a certain critical concentration, they enter a Cd2+ vacancy or a substitution with a host cation takes place. At this point the activation energy for an exchange reaction decreases dramatically near the first exchange site [3], and successively with more substitutions, igniting a cooperative reaction.

It has been suggested that the cation exchange is driven by the Coulomb forces arising from the change in the charge state of cations through the reaction pathway [3]. Since these forces should impose an atomic readjustment of atomic positions, a local strain can be supposed to appear in the reaction.
In this work we study the effect of strain on the reaction rate of the mentioned CE reaction and sketch possible technological implications.

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[2] De Trizio L, Manna L (in press) DOI: 10.1021/acs.chemrev.5b00739
[3] Florian D. Ott, Leo L. Spiegel, David J. Norris, and Steven C. Erwin
Phys. Rev. Lett. 113, 156803

Title: **Exploring point defects in the 1T' phase of single-layer MoS2**

Michele Pizzochero
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École Polytechnique Fédérale de Lausanne (EPFL)
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Abstract:
The metastable 1T' polymorph of monolayer Mo and W dichalcogenides has recently been predicted to realize the quantum spin Hall insulator phase. Furthermore, the observed coexistence of this polymorph with the stable semiconducting 2H phase results in the formation of a semimetal-semiconductor heterostructure that can potentially be exploited for realizing novel nanodevices. In the stable 2H phase point defects have widely been studied and used to tailor some relevant properties of this polymorph, such as magnetism, electronic and thermal transport as well as catalytic activity. However, the effect of point defects in the 1T' phase has not been investigated to date. Here, using first-principles methods, we fill this gap providing a complete picture of point defects in single-layer 1T'-MoS2. We consider vacancy, antisite and adatom defects, examine their thermodynamic stability, electronic and magnetic properties, both in the 1T' and 2H phase. We conclude that all considered defects have lower formation energies in 1T'-MoS2 compared to the semiconducting 2H phase. Similarly to the 2H phase, sulphur vacancies and adatoms in 1T'-MoS2 are likely to occur, while the less stable Mo adatoms and antisites trigger a magnetic response in the lattice. Contrary to the 2H phase, however, Mo vacancies are expected to be a more abundant defect, due to the structural reconstruction that takes place around the missing atom.

Title: **Origin of surprising attractive lateral interactions between oxygen adatoms on aluminum surfaces**

Matic Poberžnik
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"Jožef Stefan" Institute
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Abstract:
When electronegative atoms adsorb on a more electropositive metal surface, charge transfer occurs and adsorbed atoms become negatively charged. Because of this accumulated charge, repulsive lateral interactions are expected between the adatoms. According to the classical method of images the lateral repulsion between negatively charged adatoms can be treated as a dipole-dipole interaction that scales as Θ 3/2 , where Θ is the surface coverage of adatoms. Such dependence is typical for chemisorbed atomic oxygen on transition metal surfaces. However, in the case of O on Al(111) and Al(100) surfaces the opposite occurs and the binding energy magnitude increases with increasing coverage. Although this anomaly has been noticed, 1,2 no sound explanation as to why this occurs has been given in the literature. Hence, we attempted to explain this anomaly on a molecular level by means of DFT calculations. We found that the attractive interactions are a consequence of a simple electrostatic stabilization. Namely, at full monolayer coverage the O adatoms are located close to the surface and together with positively charged surface Al atoms form an interlaced layer of anions and cations, which is electrostatically stable. We conclude that the attractive interactions between negatively charged O adatoms at high-coverage stem from an interplay between Coulombic interactions and geometric effects, which depend on the height of adatoms above the surface.

Title: **The EPW code**

Samuel Ponce
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Abstract:

The electron-phonon interaction in the context of first-principles calculations is an often disregarded quantity due to its complexity and expected small contribution. Recent works have shown that this last assumption was incorrect and lead to a boom in the field.

The Electron-phonon Wannier (EPW) code is an open-source F90/MPI code which calculates properties related to the electron-phonon interaction using Density-Functional Perturbation Theory and Maximally Localized Wannier Functions. The code delivers Wannier interpolated electron and phonon self-energy lifetime within the Migdal approximation as well as the zero-point motion (ZPM) and temperature dependence of electronic eigenstate. The code can also be used to compute transport properties within the Migdal-Eliashberg theory.

We present the most recent developments of the EPW software: (i) the code is now fully functional with the latest version of the Quantum Espresso 6.0 software; (ii) transport properties can be calculated; (iii) anisotropic Migdal-Eliashberg theory for electron-phonon superconductors; (iv) the real part of the electron self-energy can now be computed and give access to the ZPM as well as the temperature-dependence of eigenstates; (v) tutorials and documentation have been revamped to improve user-friendly experience.

Title: **An Investigation of Group V dopants in Silicon using Linear Scaling DFT**

Jack Poulton
London Centre for Nanotechnology
London, United Kingdom

Abstract:

The aim of our work is to model the incorporation and properties of group V element dopants in silicon using linear scaling density func- tional theory. In doing so we hope to learn how to incorporate new impurities and make predictions as to how the behaviour of these im- purities for comparison with experimental data. This will then allow us to determine the suitability of certain dopants for usage as qubits in a silicon based solid state quantum computer.

Title: **Is DFT photorealistic for precious metals?**

Gianluca Prandini
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STI IMX THEOS
Lausanne

Abstract:
Gold and copper are the only two elemental metals to show a characteristic colour due to the presence of a drop of the reflectivity curve in the visible range. Reflectivities of all other metals are generally high and flat for all visible frequencies, making they appear shiny and silvery white. Nowadays, with state-of-the-art theoretical methods, it is possible to calculate colour and reflectivity of a material by means of first-principles simulations and, as a practical consequence, predict or design the colour of new alloys.

I will show and discuss results for the reflectivity and colour of several elemental metals and of some precious-metals binary alloys, considering both intermetallic and disordered compounds. Having in mind as ultimate goal the automatization of this type of simulations, the dielectric function was obtained at the simple RPA level using as starting point computationally inexpensive DFT-PBE band structures. Besides, for validation purposes, accurate convergence tests on the band structures were performed for several pseudopotential families while interpolation techniques were used to obtain the intraband contribution to the dielectric function.

This work is a first step in order to establish the computational framework for high-throughput screening of the optical properties of novel metallic alloys.

Title: **First-principles anharmonic calculations and the dynamic Jahn-Teller effect**

Joseph Prentice
TCM Group
Cavendish Laboratory
University of Cambridge
Cambridge, United Kingdom

Abstract:
First-principles density functional theory methods can be used to investigate the structural configurations, energetics and vibrational motions of solids, including anharmonicity, by using a vibrational self-consistent field (VSCF) method. The possibility of calculating an anharmonic vibrational wavefunction using this method allows anharmonic effects such as the dynamic Jahn-Teller effect to be described accurately. In this work, we apply our VSCF method to an important example of a dynamic Jahn-Teller system, the neutral vacancy in diamond. Our calculations demonstrate that the dynamic Jahn-Teller distorted tetrahedral structure of the vacancy is more stable than the static Jahn-Teller distorted tetragonal structure, in agreement with experimental observations, across a wide range of temperatures. This work opens the way for first-principles treatments of dynamic Jahn-Teller systems in condensed matter. Further examples of systems our method can be applied to are considered as well.

Title: **Magnetic susceptibility and magnetoelectric monopolization from density functional perturbation theory**

Sergei Prokhorenko
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Université de Liège
Sart Tilman, Liège
Belgium

Abstract:
Density Functional perturbation theory (DFPT) is a powerful technique that allows to calculate various physical responses including elastic, dielectric, piezoelectric, electro-optic etc. tensors from first principles. It allows the advantage of treating incommensurate perturbations while avoiding supercell calculations, and numerous application of DFPT over the past decades has proved the ability of this method to give reliable predictions of material properties.

Here, we present the treatment of linear responses to external magnetic field within the DFPT framework. Specifically, we discuss the methodology and implementation within the ABINIT package of the DFPT calculation of linear magnetic susceptibility and magnetoeletric monopolization. The implementation is tested by confronting DPFT results to finite magnetic field DFT calculations for Cr2O3. Finally, we discuss future planned developments including calculation of wave-vector and frequency resolved magnetic susceptibility and magnetoelectric tensors.

Title: **Fundamental role of defect diffusion barriers and temperature on RRAM switching mechanism**

Federico Raffone
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Dipartimento di Scienza Applicata e Tecnologia
Torino, Italy

Abstract:
Resistive switching memories (RRAM) are devices able to switch, through the application of a high voltage, among different resistive states and to retain the most recent one even when the voltage is turned off. Switching is often described in terms of charged point defect motion inside an insulating oxide under the effect of a high electric field. Such motion is a thermally activated process involving, in most cases, high diffusion barriers. In this respect, the effect of the temperature may be as important as the effect of the electric field in determining defect motion. Since Joule heating deriving from the current flowing into the oxide can lead to temperature variations, the dynamics of the defects is tremendously influenced by the occurrence of the two combined effects (voltage and heating increase). Here, we propose a mixed continuum/kinetic Monte Carlo simulation able to provide an atomistic description of the system while allowing the temperature to dynamically change during the course of the simulation so to catch all the phases of the device turn on. In this way it is possible to unveil the impact of atomic level properties, such as defect diffusivity, on higher-level quantities, like maximum reachable temperature and overall current. We will show that the temperature plays a fundamental role in triggering the resistance switching of the oxide layer in RRAM and that the switching mechanism and the device volatility change accordingly to the defect diffusion barriers.

Title: **Dynamic Covalent Bond from First Principles: Diarylbibenzofuranone Antioxidant Properties, Molecular and Electronic Structure**

Gabriel Ravanhani Schleder
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Santo André, Brazil

Abstract:

A structure that can undergo self-healing repair under standard conditions is a challenge faced nowadays, and is one of the most promising areas in smart materials science. To achieve that, the cross-linker diarylbibenzofuranone (DABBF) has been used with promising results, although without a clear comprehension of its molecular and electronic structure.

Here we use ab initio methods based on density functional theory (DFT) to fulfill this. We obtained the ground state geometry optimizations results via total energy ab initio calculations based on spin polarized density functional theory within the local density approximation (LDA), and refined the energies with the revPBE-D3(BJ) functional. We have used plane-augmented wave (PAW) pseudopotentials.

Our results indicate that the meso diasteroisomer is stable, with -1.0308 eV bond dissociation energy and 1.62 Å dynamic covalent bond lenght, longer than usual C–C bond. Oxygen interaction is weak: 0.2342 eV, compatible with physical adsorption. There is charge transfer involved in the process, with the molecule radical electron filling the oxygen pi* orbital, resulting in the superoxide, evidenced by the increased 1.277 Å O-O bond.

Antioxidant properties and structure stability is explained by electron delocalization, eletronic and molecular structure of the molecule and O2, especially the energy balance between exchange and coulomb repulsion. Thus, we described DABBF antioxidant and structural properties and its dynamic covalent bond.

Title: **Non-collinear magnetism in the Abinit Density Functional Perturbation Theory**

Fabio Ricci
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University of Liège
Liège, Belgium

Abstract:

Density functional perturbation theory (DFPT) has been widely used to compute linear response of solids with respect to atomic displacements, electric field and strain perturbations in order to get properties such as phonon dispersions, Born effective charges, dielectric constant or piezoelectric coefficients. In particular, the response of non-collinear magnets under an external solicitation is gaining a wide interest and then becoming of primary importance. In this poster, we present the generalisation of DFPT formalism to non-collinear magnetism and spin-orbit coupling. We will describe the new terms coming from the 2x2 density matrix and how we implemented this extended formalism in the Abinit code. We will show some application to non-collinear magnets where non-collinear DFPT is important to handle. This development also opens the route to compute the linear response of crystals with magnetic field perturbation to get magnetic or magneto electric susceptibilities in a systematic way.

Title: **Graphene based materials as novel membranes for water desalination and boric acid separation**

Francesca Risplendi
Politecnico of Turin
Applied Science and Technology Department
Turin, Italy

Abstract:
Desalination is one of the most promising approaches to supply water in the context of a rapidly growing global water shortage. However, the most popular water filtration method available, the reverse osmosis (RO) technique, still suffers from important drawbacks, such as a large energy demands and high process costs. In addition some serious limitations have been recently discovered; among them the low efficiency in removing boron is one of the main critical issue. Indeed, boron has been found to have a dual effect on the living systems on Earth and the difference between boron deficiency and boron toxicity levels is quite small. The aim of this project is, by means of theoretical approach based on density functional theory and classical molecular dynamics, to develop a new generation of RO membranes based on porous graphene and reduced graphene oxide able to remove salts from seawater and to reduce boron concentrations in the permeate to the level that meets the drinking or process water requirements. Computer simulations have been employed to investigate the relationship between the atomic structure of nanoporous graphene or rGO and its filtration properties in RO applications and to predict water and boric acid permeability.

Title: **NEW ADVANCEMENTS IN THE STUDY OF THE UNIFORM ELECTRON GAS WITH FULL CONFIGURATION INTERACTION QUANTUM MONTE CARLO**

Michele Ruggeri
Max Planck Institute for Solid State Research
Stuttgart, Germany

Abstract:

Full Configuration Interaction Quantum Monte Carlo (FCIQMC) [1] is able to give remarkably accurate results in the study of atoms and molecules. The study of the uniform electron gas (UEG) on the other hand has proven to be much harder, particularly in the low density regime. The source of this difficulty comes from the strong interparticle correlations that arise at low density, and essentially forbid the study of the electron gas in proximity of Wigner crystallization. We extend a previous study on the three dimensional electron gas [2] computing the energy of a fully polarized gas for N=27 electrons at high and medium density ($r_{S} = 0.5$ to 5.0). We show that even when dealing with a polarized UEG the computational cost of the study of systems with $r_{S}>5.0$ is prohibitive; in order to deal with correlations and to extend the density range that to be studied we introduce a basis of localized states and an effective transcorrelated Hamiltonian.

[1] G. H. Booth, A. J. W. Thom and A. Alavi, J. Chem. Phys. {\bf 131} 054106 (2009)
[2] J. J. Shepherd, George H. Booth and A. Alavi, J. Chem. Phys. {\bf 136} 244101 (2012)

Title: **Approximate Exchange Kernel RPA for the Condensed Phase**

Vladimir Rybkin
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Abstract:
Approximate exchange kernel (AXK) [1] random phase approximation (RPA) is beyond direct RPA approximation including exact Hartree-Fock exchange interaction, obtained by RPA-renormalization of the second-order many-body perturbation theory (MBPT2). AXK improves the redox properties as compared to the direct RPA, being applicable to small band gap systems unlike the standard MBPT2.

Here, a parallel Gamma-point implementation of RPA-AXK using the resolution-of-identity approximation for the electron repulsion integrals in the CP2K program is presented. We analyze computational scaling and benchmark the accuracy for the condensed-phase systems.

1. J . Bates and F. Furche, J. Chem. Phys. 139, 171103 (2013).

Title: **An ab initio investigation of the structural and electronic properties of Graphene Oxide**

Filippo Savazzi
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Torino, Italy

Abstract:

In recent years Graphene Oxide (GO) received particular interest, as a cheap precursor to obtain graphene as well as a functional material with tunable electronic and optical properties. Accurate ab initio studies will increase our still limited knowledge of the material, allowing for the prediction and the interpretation of experimental evidences. We studied the effects of the oxidation of graphene on its structure and electronic properties. In particular, we aimed at generating realistic theoretical models for GO and at identifying fingerprints that allow to highlight the amount and type of oxygen containing groups in GO samples. For this reason we prepared several GO structures characterised by various O/C ratio (10, 15, 20%) and with different amounts of oxygen containing groups (namely hydroxyl and epoxy groups). First we obtained a large number of samples by using classical molecular dynamics (MD) simulations, then we performed all electron density functional theory (DFT) simulations on the structures to correlate the amount and type of oxygen containing groups to variations in the Density of States (DOS). An analysis of the energy of the carbon 1s core level also highlighted that specific energy shift are found for different GO samples. This finding points at the possibility of using our results to complement and support experimental X-ray photon spectroscopy measurements.

Title: **Many-body perturbation theory - the Sternheimer-GW method**

Martin Schlipf
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Oxford, United Kingdom

Abstract:
The GW many-body perturbation method is an important tool to access accurate band gaps from first principles calculations. The conventional implementation determines the Green's function and the screened Coulomb interaction by a summation over unoccupied states tedious to converge. Giustino et al. demonstrated an alternative method to obtain these quantities by solving Sternheimer linear response equations. In this poster, we present our Sternheimer-GW software implemented in the Quantum Espresso framework and highlight some recent advances regarding the precision and stability of the method. We present our results for a small set of semiconducting materials and compare these to results obtained with conventional GW codes. We illustrate on selected examples the complete frequency dependent self energy, which is a natural product of the Sternheimer-GW method, and can be directly compared to experimental angle-resolved photoemission spectroscopy (ARPES) experiments.

Title: **Analytical integrals for fast electron correlation of periodic systems**

Patrick Seewald
University of Zurich,
Department of Chemistry
Zurich, Switzerland

Abstract:
Electron Repulsion Integrals (ERIs) are of central importance in molecular simulations and are often the bottleneck in electronic structure calculations beyond density functional theory, such as MP2, RPA and Hartree-Fock exchange. While fast methods such as Obara-Saika scheme exist, they can not be used for periodic boundary conditions. We report a new analytical scheme for periodic ERIs using a Gaussian basis. It is an analytical variant of the Gaussian and Plane Waves (GPW) method.

Title: **Dielectric-dependent Hybrid Functionals for Accurate Electronic Structure of Molecules and Periodic Systems**

Jonathan Skone
University of Chicago
Institute for Molecular Engineering
Eckhardt Research Center

Abstract:
Global dielectric-dependent hybrid (DDH) functionals were shown to yield highly accurate energy gaps and dielectric constants for a wide variety of solids, at a computational cost considerably less than standard GW calculations. The fraction of exact exchange included in the definition of DDH functionals depends (self-consistently) on the dielectric constant of the material. More recently, a range-separated (RS) version of DDH functionals where short and long-range components are matched using system dependent, non-empirical parameters was shown to yield accurate results for both finite and periodic systems. The methodology will be presented along with results using DDH functionals for several properties, including energy gaps, photoelectron spectra, absolute ionization potentials and polarization energies.

Title: **DFT-MD study of superconcentrated Li-salt electrolytes for Lithium-ion batteries**

Keitaro Sodeyama
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Center for Materials Research by Information Integration (cMI2)
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Abstract:

Li-salt concentration has been recently proposed as an important control parameter of reduction stability of electrolytes and high ion conductivity in Lithium-ion batteries. For example, highly concentrated (HC) Li-FSA salt in acetonitrile (AN) shows strong electrochemical stability against the reductive decomposition, though in low concentration (LC) solution AN is easily reduced and decomposed. However, the atomistic origin of the improved reduction stability and high ion conductivity in HC system has been still an open question. In this study, we investigated the mechanism of the improvement of the reduction stability and Li-ion diffusion mechanism depending on the salt concentration by using DFT-MD simulations. We also calculated the diffusion coefficients of the Li-ions, anions, and solvents in the LC and HC electrolytes to elucidate how Li-ion diffusion was affected by concentration. For the reduction stability, we found that TFSA anion sacrificially accepts reductive electron and decomposed in the HC systems, because specific chained network structure is formed and the electron affinity of the anion shifts lower. For the diffusion mechanism, we analyzed the motions of individual Li ions in HC system, and found Li-ion hopping between the oxygen atoms of the anions. We concluded that change of the diffusion mechanism can be an origin of the high Li-ion conductivity in the HC electrolytes.

Title: **Long-wavelength optical phonons in two-dimensional polar materials**

Thibault Sohier
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and National Centre for Computational Design and Discovery of Novel Materials
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Lausanne, Switzerland

Abstract:
Polar two-dimensional materials are bound to be used in Van-der-Waals heterostructures for next-generation electronic devices. In those materials, the treatment of longitudinal optical (LO) phonons within density-functional perturbation theory requires additional care. Indeed, in the long-wavelength limit, those phonons generate a long-ranged macroscopic electric field which proves challenging to compute. Yet, this electric field is involved in two important mechanisms that can strongly affect the performances of electronic devices. Applied to electrons, this electric field leads to the Fröhlich interaction, a strong electron-phonon coupling. Applied to the dipoles induced by the LO phonons themselves, it leads to the so-called LO-TO splitting. While methods have been developed to treat those phenomena in three-dimensional materials, direct ab initio calculations and detailed models are still lacking in the two-dimensional case. Due to the involvement of screening and the long-range Coulomb interaction, LO-TO splitting and Fröhlich interactions cannot be treated in the usual three-dimensional periodic-boundary-conditions framework. We use a truncated Coulomb interaction [1] to perform density-functional perturbation theory calculations in a two-dimensional framework. We present extensive simulations and detailed models of LO-TO splitting [2] and the Fröhlich [3] interaction in various two-dimensional systems, including materials such as transition-metal dichalcogenides, indium chalcogenides and hexagonal boron nitride.

[1] T. Sohier, Electrons and phonons in graphene : electron-phonon coupling, screening and transport in the
field effect setup, PhD thesis, Universite Pierre et Marie Curie, Paris VI (2015).
[2] T. Sohier, M. Gibertini, M. Calandra, F. Mauri, and N. Marzari, in preparation (2016).
[3] T. Sohier, M. Calandra, and F. Mauri, Physical Review B 94, 085415 (2016).

Title: **DensToolKit: A comprehensive open-source package for analyzing the electron density and its derivative scalar and vector fields. Current developments**.

Juan Manuel Solano Altamirano
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Meritorious Autonomous University of Puebla
Puebla, Mexico

Abstract:
DensToolKit is a suite of open-source programs for analysing the electron density [ED] as well as other fields derived from it. The suite includes different tools for analysing the fields using traditional methods such as creating grids in 0-, 1-, 2- and 3-dimensions, but it includes other tools for analyising the topology of the ED, including trajectory integrals over bond paths (to the best of our knowledge this is a feature unique to DensToolKit, and we are currently working on possible applications). DensToolKit includes programs for analysing densities in spaces other than the position as well, for instance it can analyse electron density in momentum space (and fields such as the kinetic energy in this space), as well as programs to analyse the density matrix of order 1 both the scalar field and its gradient. The versatility of the suite can be further extended because it follows the guidelines of the Object Oriented Programming paradigm in its design, and we are currently working on a re-design that will allow to include more methods for computing the electron density, and consequently, the possibility of analysing more systems, especially for carrying out the topological analysis of the electron density in Materials Science related systems.

Title: **Electronic Properties of Organometallic Graphyne Networks on Ag(111)**

Himadriben R. Soni
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Abstract:
Graphyne and graphdiynes are two dimensional carbon allotropes consisting of sp2 and sp- hybridized carbon atoms. Various types of graphynes have been suggested by inserting carbon triple bonds (−C≡C−) into C−C bonds of graphene. Some graphynes and graphdiynes contain band structures with Dirac points and thus are interesting for next-generation nano- electronic devices. Herein, we present the electronic structure of newly synthesized, two-dimensional, surface-supported organometallic graphynes, using density-functional theory (DFT) calculations. Specifically designed Br-substituted triethynyl-derivatives were used as precursor molecules to fabricate porous organometallic Ag-acetylide after cleavage of the C-Br bonds on Ag(111). In addition, a chemical modification of the precursor allows us to investigate the effect of Nitrogen doping in our two-dimensional carbon networks. Scanning tunneling spectroscopy reveals unoccupied electronic states that are delocalized along the organometallic graphyne on Ag(111). The latter, as well as the electronic structure of the organometallic graphynes, are further analyzed by DFT calculations, revealing that the metall-bis-acetylide bonds are metalor- ganic bonds with ionic character.

Title: **Planar versus three-dimensional growth of metal nanostructures at graphene**

Srdjan Stavric
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Vinca Institute of Nuclear Sciences,
Laboratory for Theoretical and Condensed Matter Physics
Belgrade, Serbia

Abstract:
Employing density functional theory we studied microscopic mechanisms governing initial stages of growth of three selected metals (Li, Ti and Ca) on graphene.Tendency towards planar or three-dimensional (3D) growth is rationalized based on atomic-scale description of the interaction between metal adatoms, as well as adsorption geometries of their trimers and tetramers. Li atoms, featuring a long-ranged electrostatic repulsion, are individually dispersed across the surface, in a sharp contrast with atoms of transition metal Ti which gather into densely-packed 3D clusters due to a strong short-ranged metal-metal attraction. Modest attractive interaction between Ca adsobates enable formation of monoatomic films with the local coverage of 1/6 monolayer – structure with great stability and high density of states at Fermi level.

Title: **Tunable quantum conductance in MoS2 nanoribbons**

Fatemeh Tabatabaei
Department of Physics
Isfahan University of Technology
Isfahan, Iran

Abstract: NO TEXT - I copied the description of her research.

I'm investigating quantum transport in MoS2 nanoribbons. Our first-principle calculations are performed utilizing Quantum-Espresso package and the wannierization is obtained by Marzari and vanderbilt's method using the WANNIER90 code.Also I'm investigating strain effect and adsorb different gases on quantum transport. I'm wondering is there any MoS2 nanoribbons that can be used for gas sensor? or for some pressure sensor?

Title: **Effects of dopants different configurations on electronic structure and magnetic properties of N-doped graphene: an ab-initio study**

Yavar Taghipour Azar
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Physics and accelerator school
Atomic Energy Organization of Iran, AEOI
Teran, Iran

Abstract:

All possible bonding configurations of N dopants in carbon network can be classified into three main categories: graphitic, pyridinic, and pyrrolic N. Taking into account possible magnetization of these structures, electronic structure of all doped systems have been calculated in spin-polarized DFT framework. Our results predict almost zero magnetization for graphitic N-doped graphene, and relatively small value (~0.1) for pyridinic systems, where pyrrolic N can create a significant difference between the spin up and down densities and also, localized magnetization around pyrrolic nitrogen. These distinguished results for pyrrolic N-doped graphene suggest it as an attractive material for spintronic and catalytic applications.

Title: **Graphene trumpets, foams, pillared networks, carbon materials growth, and all that from first-principles and classical molecular dynamics simulations**

Simone Taioli
European Centre for Theoretical Studies in Nuclear Physics and Related Areas
Trento, Italy

Abstract:
I will discuss first the processes leading to the room-temperature growth of carbon based nanocrystals, notably silicon carbide (SiC) and graphene, by supersonic molecular beam epitaxy. In particular, I will present both experiments and computational modeling of fullerene impacts on silicon and copper surfaces at intermediate-energy regimes (few tens of eV). This collision induces strong chemical-physical perturbations in the system and, for sufficient C60 translational energy, disruption of molecular bonds and cage breaking. This mechanism can lead to the formation of nanostructures with different stoichiometric character. Characterization of the epitaxial grown material by a variety of experimental techniques, such as XPS, UPS, Auger, LEED, TEM, and Raman after the collision, demonstrates the potentiality of our approach to grow nanostructured materials at room temperature. On the theoretical side, we show that in these out-of-equilibrium conditions, it is necessary to go beyond the standard implementations of ab-initio molecular dynamics, as ab-initio methods based on the Born-Oppenheimer approximation fail to capture the excited-state . In particular, we analyse the Si- and Cu-C60 collision within the non-adiabatic nuclear dynamics framework, where stochastic hops occur between adiabatic surfaces calculated via time-dependent density functional theory. The theoretical description of C60 impacts on metallic and semiconductor substrates is in good agreement with our experimental findings. Finally, applications of molecular dynamics and classical minimization techniques to describe the mechanical properties of carbon-based nano-foams, the discovery of a novel energetically stable carbon structure shaped as a Beltrami pseudosphere, and the gas-sieving properties of pillared graphene oxides will be shown.

Title: **ZnO Nanoporous: Structural and Electronic Study Under Elastic Strain**

Alvaro David Torrez Baptista
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Santo André, Brazil

Abstract:

One of the most important topics of material science research is the investigation of nanostructured materials, due to the possibility to obtain the best of the quantum confinement effect applicability in different areas. The ZnO have attracted attention because of its properties with potential applications on optical devices, transparent contacts, enhancement structures for light emitting diodes (LED's), transparent thin films transistors, transducers, among others.

Using structural modifications is possible to alter and control the properties of materials. Obtaining porous structures is an area of intense research. Currently, there are several experimental techniques for this purpose. Another possibility is the application of elastic strain to tune the physical and chemical properties of different kind of materials.

We investigated a zinc oxide nanoporous under biaxial elastic strain through first-principles methods based on total energy ab initio calculations. We have used spin-polarized Density Functional Theory within the Generalized Gradient Approximation (GGA).

Our results show that the elastic strain leads to a non-uniform distribution charge localization in the surface of the nanoporous. Using a biaxial tension above 4%, of the ZnO bulk lattice parameter, we observe a phase change region in the structure. Our results show that the values of band gap are tuned by the strain with an opposite trend observed for the bulk.

Title: **High-Throughput Generation and Analysis of a Large Dataset of Organic/Inorganic Hybrid Perovskites**

Huan Tran
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Abstract:

Organic/inorganic hybrid perovskites are particularly promising materials for photovoltaic applications with an efficiency of more than 20%. While methylamonium-containing perovskites, e.g., CH3NH3PbI3 and CH3NH3SnI3, are of primary interest, the hybrid perovskite family is significantly diverse in terms of both the possible organic cations [1] and the structural motifs [2]. To accelerate the exploration of this family by emerging computational methods, we develop a dataset of more than 1,000 low-energy structures of organic/inorganic halide perovskites, containing 16 possible organic cations [3]. The structures in this dataset are determined by combining density functional theory computations with the minima-hopping structure predictions method. The band gaps of these hybrid perovskites are calculated at the HSE06 level [4], enabling a direct comparison with the experimental data. We will discuss the preparation of the dataset, our analysis and some insights that emerged from it.

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Title: **First-principles calculation on rare earth doped tellurides: thermoelectric and magnetic properties**

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Abstract:
Bismuth telluride with doped magnetic elements have been great of interest in the years due to its potential application as thermoelectric materials and its unique electronic structures related to the topological insulator. Rare earth doping reveals many exotic magnetic property change in host materials. In this work, within the density functional theory, we perform first-principles electronic structure calculation by employing the all-electron full-potential linearized augmented planewave (FLAPW) method [1] to examine magnetic properties and thermoelectric properties of rare earth doped bismuth telluride. The strong correlation and spin-orbital coupling effects are crucial to describe the electronic structure of the compound. Results show that rare earth substituted Bi2Te3 compound is magnetic alignment with the magnetic moment purely from f-states of rare earth atoms. Interaction between the valence electrons produces a semimetallic feature, which reduce drastically the Seebeck coefficient. To substantiate, we calculate the Seebeck coefficient, the electrical conductivity, and the thermoelectric power factor by utilizing the solution of Boltzmann transport equation in a constant relaxation-time approximation and make discussions to improve the TE performance of the compound.

Title: **Probing the electronic structure for 3d-3p and 3d-3s hybridized states using resonance photo-emission spectroscopy**

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Abstract:

SmCrO3 is a newly emerging compound due to the abrupt spin reorientation phase transition and multiferroic properties making it a potential candidate for ultrafast spin switching to modify recording media and thermo-magnetic power generation. The origin of magnetic and electrical behavior of a material is always intrinsically correlated with the electronic structure and thus the study of valence band has been of fundamental scientific interest. In the present work we probe the valance band of SmCrO3 using resonant photoemission spectroscopy (RPES) technique with variable photon energy provided by synchrotron source. In the present study, for RPES measurement, incident photon energies are varied from hυ = 40-80eV which covers the chromium 3p->3d and 3s->3d excitation thresholds to observe the resonance like enhancement in photoemission intensity profile. The constant initial state plots are constructed to analyze the photon energy dependent behavior of the features of valence band spectra. The presence of two resonance like enhancement in intensity profile of oxygen feature in valence band spectra reveal the strong hybridization of Cr-3d and O-2p orbital. The origin of the resonance like feature at 51eV can be explained on basis of the interference of two possible channels for photoemissions: one due to direct photoemission from 3d state, and the second due to absorption of photon by 3p state followed by super Kroster -kronig decay. The secondary maximum observed at high photon energy is expected due to charge transfer excitation from 3s core level -> 3d valence band assisted by a hybridized ligand environment.

Title: **Current-induced orbital magnetism in doped tellurium.**

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Abstract:

Noncentrosymmetric conductors belonging to the gyrotropic crystal classes become magnetized while carrying a current [1,2]. Contrary to the more familiar magnetoelectric effect in insulators, this "kinetic magnetoelectric effect" does not require a magnetically-ordered ground state. Moreover, spin-orbit coupling is only needed to generate a spin magnetization (the "Edelstein effect"), but not for the orbital part. We have calculated from first-principles the magnetization induced in doped tellurium by a current propagating along the trigonal z axis, as well as the accompanying anomalous Hall effect, and the Faraday rotation, measured in experiment [3]. For the experimental values of doping concentration p = 4x10^{16} cm^{-3} and a current j = 10^3 A/cm^2 the orbital moment m_z and anomalous Hall conductivity sigma_xy are comparable to those occuring spontaneously in ferromagnetic iron, while the induced spin moment is much smaller than the orbital part.

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Title: **First-Principles Study of The Electronic Structure in Molecular Conductors with Hybrid Functional**

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Abstract:

Molecular conductors show a rich variety of ground states such as antiferromagnetic state, quantum spin liquid, superconductivity, charge ordering, spin-density wave ordering, spin-Peierls state, and so on. Such a richness of properties originates from relatively large Coulomb interactions. Simple tight-binding models have been proposed for explaining these phenomena qualitatively, but quantitative evaluation of physical quantities and understanding of microscopic picture between different phases remain challenging. To obtain reliable picture of the electronic states by first-principles density functional theory (DFT) calculations, computational approaches that can be applicable for molecular systems with a reasonable cost are highly required. We study the molecular conductors showing charge ordering and antiferromagnetic state, and apply the hybrid functional approach with Heyd-Scuseria-Ernzerhof functional. The formalism enables us to improve the exchange correlation energy by mixing the non-local exact (Fock) exchange and (semi) local exchange energy functional used in conventional DFT approaches such as LDA or GGA. We will discuss systems such as quasi-one-dimensional (TMTTF)2X where X = PF6 and AsF6, quasi-two-dimensional α-(BEDT-TTF)2I3, and hydrogen bonded system κ-H/D3(Cat-EDT-TTF)2.

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Title: **Delivering on the promises of high-throughput atomistic simulations using verification, data provenance and workflows**

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Abstract

High-throughput approaches have established themselves as a cornerstone of materials discovery and understanding. Within MARVEL we adopt a hierarchical approach split into three tiers. At the bottom are the atomic simulation codes, usually electronic structure theory. The middle tier consists of a database-backed, provenance tracking and automation engine that unifies the submission of calculations across different codes and computational resources, keeping track of the full provenance of any result. The last tier consists of an easy to use, yet powerful, workflow engine that allows experts to encode their knowledge and decision making to automate common tasks and make sophisticated calculations accessible to non-experts. These final two tiers are implemented in the AiiDA Python platform.

To demonstrate the enabling power of AiiDA I will present result from a project aimed to complete our knowledge of (low lying) binary (DFT) inorganic compounds (with reasonable number of atoms in the primitive unit cell). In this work we use the Pauling File, an extensive database of experimental crystal structures and properties, as a reference and calculate the energies and basic properties for all relevant compounds therein, spanning over 13,000 distinct solids. In this first step these results are used to validate the accuracy of DFT while in the second we go beyond the known compounds and fill in the gaps by using ionic substitution in the commonly occurring prototypes to explore compounds that have not been reported in experiment. I will focus on the technologies and worflows that enable such large scale calculations.

Title: **Anisotropic thermal conductivity of arsenene and phosphorene: An ab initio study**

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Abstract

Elemental two-dimensional (2D) materials exhibit intriguing heat transport and phononic properties. Here we have investigated the lattice thermal conductivity of newly proposed arsenene and phosphorene, using ab initio calculations. Solving the Boltzmann transport equation for phonons, we predict a highly anisotropic thermal conductivities along the zigzag and armchair directions, at room temperature. Our calculations reveal that phonons with mean free paths between 20 nm and 1μm provide the main contribution to the large thermal conductivity in the zigzag direction in arsenen; mean free paths of phonons contributing to heat transport in the armchair directions range between 20 and 100 nm. The obtained anisotropic thermal conductivity and feasibility of synthesis, in addition to high electron mobility reported elsewhere, make arsenene a promising material for nanoelectronic applications and thermal management.

Title: **Modeling the FePc adsorption on the moire superstructure of graphene intercalated with a Co layer**

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Abstract

The moiré superstructure of graphene grown on metals can drive the assembly of molecular architectures, as iron-phthalocyanine (FePc) molecules, allowing for the production of artificial molecular configurations. A detailed analysis of the Gr/Co interaction upon intercalation (including a modelling of the resulting moiré pattern) is performed here by density functional theory, which provides an accurate description of the template as a function of the corrugation parameters.

In particular, the chemical shifts of carbon atoms for Gr/Ir intercalated with a Co monolayer have been studied by means of first principle calculations, allowing a sound interpretation of the two-peaked structure of XPS spectra recently measured in terms of corrugation and hybridization of the graphene layer. The description of graphene corrugation requires a large unit cell. Based on previous results for Gr/Re(0001), we successfully used a model for the moiré patterning which permitted to simulate the actual XPS C1s energy splitting without explicitly performing a calculation for each of the 200 C atoms, lowering considerably the computational cost. The theoretical results are a preliminary step to describe the interaction process of the FePc molecules adsorption on the Gr/Co system.

Title: **Nanotherm: Ab initio integrated tool to describe thermoelectricity {in nanostructures from materials to devices**

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Abstract:
Thermoelectric devices enable the direct and reciprocal conversion between thermal and electric energy, offering solutions for generation of electrical power, energy recycling, heat management in nanoelectronic devices and conversion of waste heat lost. Energy conversion \textit{via} the thermoelectric effect is thus a topic of tremendous interest in materials science, and an increase of the material efficiency -measured by the thermoelectric figure of merit ZT- is actively searched for by nanostructuring. Indeed, downsizing sample size induces reduction of the thermal conductivity κ, and consequently increases ZT, which is inversely proportional to κ. Improving the efficiency of thermoelectric materials requires a deep understanding of the mechanisms that control both electronic and heat transport. In the Nanotherm project, our studies in silicon, bismuth and germanium, aim at investigating the conditions for which thermoelectricity efficiency can be improved.

In particular, we will show the influence of nanostructure size and shape on the thermoelectric coefficient of silicon, on the thermal conductivity of silicon [1] and bismuth [2,3], as well as preliminary results on germanium. Our study involves the computation, on the quantum level, of phonon-phonon interaction and electron-phonon coupling from first principles, \textit{i.e.} without adjustable parameters. We underline the importance, in a device-oriented perspective, to combine different computational techniques (\textit{ab-initio} and Monte Carlo). I present also an example of thermo-device designing by using molecular dynamics simulations in the case of graphene [4].\\
The Nanotherm project [5] is performed in collaboration with J\'er\^ome Saint-Martin and Philippe Dollfuss, C2N, Universit\'e Paris Sud, Orsay.

Title: **Encapsulated Nanowires: Boosting Electronic Transport in Carbon Nanotubes**

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Abstract

Carbon Nanotubes (CNTs) are the most promising candidates for nanoelectronic conductors due to their excellent electrical conductivity [1-3]. However experimental and theoretical studies show that electronic transport in metallic CNTs undergoes a dramatic decrease beyond a bias of ~0.2eV due to scattering of conduction electrons from a population of high frequency phonons [4-7]. Under bias voltage, the hot phonons constitute the dominant source of electron scattering, and hence resistivity, in metallic CNTs. A mechanism for increasing the rate of phonon thermalisation will therefore enhance the electrical performance of CNTs.

The process of phonon deexcitation involves anharmonic phonon-phonon scattering, hence its rate is dependent on the number of available channels for phonon decay. We demonstrate from first principles that reduction of the hot phonon population under bias is readily achievable via encapsulation of 1D nanowires in single-walled CNTs (SWCNT). We show that an encapsulated one-dimensional crystal creates additional channels for hot phonon thermalisation, increasing the decay rate. Pacification of the phonon population growth reduces electrical resistivity of metallic CNTs by 34% for an example system with encapsulated beryllium.

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Title: **Invisible Gold Adatoms and where to find them: the case of Dimethyl Sulfoxide on a Gold Surface**

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Abstract

We report the formation of dimethyl sulfoxide (DMSO) molecular complexes on Au(111) enabled by native gold adatoms unusually linking the molecules via a bonding of ionic nature, yielding a mutual stabilization between molecules and adatom(s). DMSO is a widely used polar, aprotic solvent whose interaction with metal surfaces is not fully understood. By combining X-ray photoelectron spectroscopy, low temperature scanning tunneling microscopy, and density functional theory (DFT) calculations, we show that DMSO molecules form complexes made by up to four molecules arranged with adjacent oxygen terminations. DFT calculations reveal that most of the observed structures are accurately reproduced if, and only if, the negatively charged oxygen terminations are linked by one or two positively charged Au adatoms. A similar behavior was previously observed only in nonstoichiometric organic salt layers, fabricated using linkage alkali atoms and strongly electronegative molecules. These findings suggest a motif for anchoring organic adlayers of polar molecules on metal substrates and also provide nanoscale insight into the interaction of DMSO with gold.

Title: **Cubic scaling RPA correlation energy calculations**

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Abstract

The random phase approximation (RPA) for computing the electron correlation energy has emerged as an accurate tool for predicting the properties of molecules and condensed phase systems. RPA combines a number of attractive features, most importantly that long-range van der Waals interaction is included, in contrast to semilocal density functionals. The drawback connected with RPA is the computational cost: For canonical implementations of RPA, the numerical effort grows as quickly as O(N4) with the system size N. We present a new algorithm for computing the RPA correlation energy in a Gaussian basis requiring O(N3) operations and O(N2) memory. The cubic-scaling RPA method is based on the resolution of the identity (RI) with the overlap metric, a reformulation of RI-RPA in the Gaussian basis and imaginary time as well as the use of sparse linear algebra. We report a massively parallel implementation which is the key for the application to large systems. As first benchmark of the method, we show the RPA correlation energy of thousands of water molecules in a high-quality cc-TZVP basis. For a comparison, the canonical RPA method is restricted to 500 water molecules using the whole Piz Daint supercomputer for two hours. Our new RPA algorithm enables the application of RPA to large systems where van der Waals interactions play an important role, e.g. for predicting the adsorption energy of large molecules on surfaces.

Title: **Oxygen reduction reaction on the defective tetragonal ZrO2(101) surface**

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Abstract

For future polymer electrolyte fuel cells (PEFCs), ZrO2 has attracted much attention as a durable and inexpensive electrocatalyst [1]. Although its oxygen reduction reaction (ORR) activity becomes comparable to platinum by introducing oxygen vacancies (Vos) and impurities such as C and N atoms, their role is unidentified experimentally. Theoretically, elucidating the ORR activity at a defective oxide surface is a major challenge. In this context, we have attacked this problem with first-principles density functional calculations of the tetragonal ZrO2(101) surface taking the effects of adsorbed water molecules and defects into accounts. By investigating various adsorbed configurations of water molecules, we have found that the surface structure is much more complex than has been thought based on a previous calculation [3]. The pristine surface adsorbed by water molecules is not reactive against ORR because the adsorptions of intermediates are too weak. Introducing a Vo and N atoms at the subsurface strengthens the adsorptions, but the surface remains non-reactive. On the other hand, the surface becomes reactive when introduced with the defects at the surface according to our free-energy diagram of ORR. Our calculation suggests that the defective surface is activated at the surface oxygen vacancy but not at the surface Zr site, exhibiting unconventional catalytic property.

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Title: **Optical fingerprints of solid-liquid interfaces: a joint ATIR and first principles investigation**

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Abstract

Despite the importance of understanding the structural and bonding properties of solid-liquid interfaces for a wide range of (photo-)electrochemical applications, there are presently no experimental techniques available to directly probe the microscopic structure of solid-liquid interfaces. We carried out joint ATR-IR spectroscopy measurements and ab initio molecular dynamics simulations of the vibrational properties of interfaces between liquid water and prototypical semiconductor substrates. In particular, the Ge(100)/H2O interface is shown to feature a reversible bias potential dependent surface phase transition. Our study highlights the key role of coupled theory-experimental investigations on well controlled and characterized interfaces, in order to develop robust strategies to interpret experiments and validate theory. G. Galli. and F. Gygi. acknowledge DOE-BES Grant No. DE-SS0008939.

Title: **High temperature thermoelectric study on Zr and Hf based transition metal dichalcogenides**

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Abstract

We investigate the electronic and thermal transport properties of bulk transition metal dichalcogenides, MX2 (M = Zr, Hf and X = S, Se) by first-principles calculations and semi-classical Boltzmann transport theory. The band structure of these compounds show the confinement of heavy and light bands along the out of plane and in-plane directions, respectively. This results in high electrical conductivity and large thermopower leading to a high power factor for moderate n-type doping. The phonon dispersion demonstrates low frequency flat acoustical modes, which results in low group velocities. Consequently, lowering the lattice thermal conductivity below 2 W/m K. Low κ latt combined with high power factor results in ZT > 0.8 for all the bulk MX2 compounds at high temperature of 1200 K. In particular, the maximum ZT of HfSe 2 exceeds 1 at 1400 K, which shows higher performance than SiGe. Our results show that Hf/Zr based dichalcogenides are very promising for high temperature thermoelectric application.

Title: **Temperature effects on the relative stability of ultra-high pressure phases of oxygen**

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Abstract

Recent technical developments in ramp-compression experiments have enabled researchers to take systems to very high pressures at relatively low temperatures, this permits the study of very dense systems that are still in their solid phase and can undergo solid to solid phase transitions. Calculations in oxygen have predicted a phase transition from a molecular to a fully extended solid phase at pressures above 9TPa. Those calculations were performed at zero temperature. Here we analyse the transition to a non-molecular oxygen phase including temperature effects, and study the implications of our results on the feasibility of carrying out future experiments aimed to studying this transition with the currently available techniques.

Title: Simulations of water nano-confined between corrugated planes

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Water confined to nanoscale widths in two-dimensions between ideal planar walls has been the subject of ample study, aiming at understanding the response of water to confinement without the consideration of the chemistry of actual confining materials. In this work, we study the response of water to the imposition of a periodicity in the confinement by computer simulations, using both empirical potentials and first-principles calculations. For that we propose a periodic confining potential that allows varying the lattice parameter and amplitude of the oscillation. We do it for a triangular lattice, with several values of the lattice parameter: one which is ideal for commensuration with layers of Ih ice, and other values that would correspond to more realistic substrates. For the former, the obtained phase diagrams show an overall rise of the melting temperature as should be expected. For the latter, although the liquid does not freeze, it is observed to be more structured and follow the valleys of the potential. By calculating both the free energy and enthalpy of confinement, we can confirm that the main factor in the resistance of water to be confined is entropy. The introduction of the modulation lowers the internal energy of the confined water with respect to that for flat confinement, but the modulation originates a free energy rise at room temperature due to the decrease in entropy induced by the modulation. The used empirical potentials (TIP4P/2005) and the first principles simulations agree in the main conclusions of this study, except for the interlayer vertical correlation, which is very substantially suppressed by the modulation, while the classical water is only mildly affected.

Ttitle: **GW calculations of anatase TiO2 systems of different dimensionality**

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Abstract

Titaniun dioxide (TiO2) is a relevant material for photocatalysis and solar cell conversion. In this poster we present results obtained in the study of electronic properties of anatase TiO2 systems of different dimensionality, from bulk to nanocrystals. Electronic properties are calculated by combining the QE-package with a new version of the Yambo code where new routines are implemented to reduce the number of empty states necessary to converge GW calculations. The dependence of electronic properties on the size, shape and dimensionality of the systems will be analyzed and discussed in detail.

Title: **The microscopic dynamics of ABO3 perovskites**

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Abstract

Ferroelectric materials like BaTiO3 have been used for decades in a broad range of technological applications (capacitors, gate dielectrics, IR detectors, holographic memories, ...). However, there is still significant debate concerning the microscopic behaviour of these materials, in particular near the paraelectric–ferroelectric phase transition. BaTiO3 and KNbO3, for instance, display a complex energy landscape with B-cations (Ti or Nb) displacing with respect to the center of the oxygen cage and thus creating local dipole moments even in the cubic paraelectric phase. Models such the eight-site model have been developed in the literature to explain the experimental findings. In order to clarify the microscopic behaviour of these materials, we first perform a large set of ab-initio molecular dynamics calculations to assess the driving mechanisms for the local non-collinear displacements in the high-temperature phases. We then use spacegroup techniques to systematically investigate the energy landscape of these perovskites and analyse all possible local displacement patterns that are compatible with a net paraelectric phase. These are followed by total-energy DFT calculations to check the energetics and the stability of these patterns. Using this technique, we are able to identify descriptors for the occurrence of the local ferroelectric dipoles, that we can correlate with the finite-temperature MD simulations and use to systematically explore the energy landscape of a set of representative ABO3 perovskites.

Work done in collaboration with A. Cepellotti (EPFL), S. Halilov (MIT), B. Kozinsky (Bosch RTC), M. Fornari (Central Michigan University), N. Marzari (EPFL).

Title: **Charge localization and energetics of Li-ion batteries cathodes from extended Hubbard-corrected functionals**

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Abstract

The accurate modeling of the electronic, magnetic and structural properties of transition-metal (TM) compounds is essential for the development of several emerging technologies. Unfortunately, the importance of electronic correlations impairs significantly first-principles calculations on these systems. This is also true for many materials being explored for the electrodes of Li-ion batteries. In fact, most approximate energy functionals fail capturing the localization of valence electrons on TM ions during the charge/discharge transients thus compromising the energetic modeling of these systems and the assessment of their performance.

Hubbard-model augmented DFT functionals (DFT+U) improve significantly the description of correlated materials and have asserted themselves as the standard choice to the modeling of these systems when high computational efficiency is required (e.g., for screening large numbers of compounds). This work shows how an extended formulation of DFT+U, including on-site (U) and inter-site (V) interactions, improves the description of mixed valence materials. Focusing on LixMPO4 (M = Fe, Mn, Ni, Co) we discuss their equilibrium structure and electronic properties in dependence of Li content. Contradicting a common practice, we also show that using computed interaction parameters is actually crucial to reliably compare the energy of different Li concentrations and, in particular, to assess the thermodynamic stability of intermediate compositions and to evaluate the voltage of the resulting battery.

Title: **Hubbard interactions from density-functional perturbation theory**

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Abstract

DFT + U, together with its V and J extensions, is a simple and powerful tool to model systems containing partially-filled manifolds of localized states [1]. However, the Hubbard parameters are often - and in our view incorrectly - treated semi-empirically. Conceptual and practical methods to determine e.g. the Hubbard U parameter have nevertheless been introduced long ago, based either on the constrained random-phase approximation (cRPA) [2] or on linear-response theory [3]. These approaches make DFT+U a fully first-principles and self-contained method, but are often overlooked due to their cost or complexity. Here, we introduce a computationally inexpensive and straightforward approach to determine the linear-response U, hitherto obtained from the difference between bare and self-consistent inverse electronic susceptibilities evaluated from supercell calculations. By recasting these calculations in the language of density-functional perturbation theory [4] we remove the need of supercells, and allow for a fully automated determination of susceptibilities and Hubbard parameters. Such developments open the way for deployment in high-throughput studies, while providing the community with a simple tool to calculate consistent values of U for any system at hand. Last, the approach is showcased with applications to selected transition-metal compounds.

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Ttiel: **Simulations of electron energy loss spectra with turboEELS: preliminary results**

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Abstract

Plasmonics is a rapidly developing branch of nanophysics, as it proposes a variety of tools that can be used both in research and industry (i.e. plasmonic waveguides, near field microscopes, surface plasmon resonance sensors, etc), so plasmons and their properties have been extensively studied during last decades both experimentally and theoretically.

From the theoretical point of view it is necessary to have a tool that allows to characterise and study plasmons in an accurate and efficient way. In this project we use the Liouville-Lanczos algorithm implemented in the turboEELS code [1] of Quantum ESPRESSO. We compute the electronic susceptibility in time-dependent density functional perturbation theory (TDDFPT) and simulate electron energy loss spectra (EELS) in order to study surface plasmons in noble metals (Au, Ag, Cu) with the main focus on gold surfaces.

In previous studies of surface plasmons in Au, spin-orbit coupling was not taken into the account [2], while it is known that this effect influences band structure significantly. In our project we would like to emphasise the importance of spin-orbit coupling and to perform full relativistic study of EEL spectra for Au surfaces. In particular, we have already shown that there is non-negligible difference between EELS of bulk Au with and without spin-orbit coupling. In order to perform the efficient study we are implementing the spin-orbit coupling interaction with ultrasoft pseudopotentials in the turboEELS code.

Performance of the turboEELS code will also be presented on bismuth [3] and on silicon.

We thank Iurii Timrov, Tommaso Gorni and Stefano Baroni for fruitful discussions.
Support from the DGA is gratefully acknowledged. Computer time was granted by Ecole Polytechnique through the LLRLSIproject and by GENCI (Project No. 2210).

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