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P01

Tricking germanium to open the band gap

An efficient method to open the band gap of germanium is presented in detail. The methods works by ad- justing the Kohn-Sham Hamiltonian under the framework of density functional theory. A functional that de- cays faster than the pseudopotential wave function was projected on the 4s-orbital thereby increasing the energy of the system. Exact experimental direct band gap (0.81eV) of germanium at room temperature was obtained. For the indirect band gap, 0.67 eV was obtained, which is very close to the experimental band gap of 0.66 eV. Finally, with our new approach, vacancy in germanium was found to have an acceptor level at E V + 0.4 eV which is quite close to the experimental observation of E V + 0.33 eV.

Atomic scale nucleation and formation mechanism of hexagonal boron nitride (hBN) on graphene and Germanium : A DFT study

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Abstract

Hexagonal boron nitride (hBN), as an important member of two-dimensional (2D) materials has received great attention recently owing to its exciting optoelectronic properties combined with high thermal conductivity and chemical stability. It is also an ideal material to isolate other 2D materials, including graphene, from the substrate or from the environment. The synthesis of high-quality h-BN over a large area of various substrate is highly desired. However, finding an appropriate the growth condition remains challenging. We focus our investigation on graphene for the importance of its intrinsic transport properties that can only be obtain for isolated layer and on germanium substrate for its compatibility with silicon technology. To understand the nucleation path of hBN growth on graphene, Ge(100) and Ge(111) by chemical vapor deposition (CVD) and Molecular Beam Epitaxy (MBE), we systematically investigated the adsorption, formation energy and the stability of atomic B and N as well as hBN clusters using density functional theory (DFT). Interestingly, the results reveal that B atoms could be easily adsorbed on three identical sites with strong bounding on Graphene and Ge(100) surfaces while its prefer the fcc site on Ge(111), whereas the N atoms prefer the top on Ge atoms and the bridge site when it is adsorbed on Ge(100) and Ge(111), respectively. The diffusion barriers for the B and N atoms were calculated by the climbing nudged elastic band (c-NEB) method; B and N atoms diffuse almost freely on graphene surface. However, a high diffusion barrier was observed for both the B and N atoms on the Ge(100) and Ge(111) surfaces indicating that the surface diffusion is more competitive. Different geometries of hBN clusters were also studied; we systematically investigated the alignments of triangular BN clusters on graphene surface. Finding that the stability and formation energy increase with increasing BN chains on Germanium, with the addition of B-N pair, the formation energies become more energetically favorable and ring chains are likely formed from linear chains. Hence, we believe that this finding could be useful in understanding the growth mechanism of hBN and will motivate further experimental designs in CVD and MBE growth of hBN.

Keywords: 2D materials, hBN growth, Graphene, Adsorption, c-NEB, DFT.

P03

Insights from density functional theory into the formation and rotation of an enantiospecific assembly of molecular raffle wheels

Tailored nano-spaces can control enantioselective adsorption and molecular motion. We report on the spontaneous assembly of a dynamic one-component system - a rigid kagome network with each pore occupied by a guest molecule - employing solely 2,6-bis(1H-pyrazol-1-yl) pyridine-4- carboxylic acid on Ag (111). The network cavity snugly hosts the guest, bestows enantiomorphic adsorption, and allows selective rotational motions. Temperature-dependent scanning tunneling microscopy studies revealed distinct anchoring orientations of the guest unit switching with a 0.95 eV thermal barrier. H-bonding between the guest and the host transiently stabilizes the rotating guest, as the flapper on a raffle wheel. Density functional theory investigations unravel the detailed molecular pirouette of the guest and how the energy landscape is determined by H-bond formation and breakage. The origin of the guest's enantiodirected, dynamic anchoring lies in the specific interplay of the kagome network and the silver surface.

P04

Floquet Theory of Electronic Stopping of nuclei projectiles in solids

Floquet Theory of Electronic Stopping of nuclei projectiles in solids Authors: Marjan Famili, Nicolo Forcellini, Jessica Halliday and Emilio Artacho Nuclei shooting through solids give rise to strongly non-equilibrium processes among electrons in solids, which have been studied in different ways for decades due to their interest as prototipical quantum dynamical problems, but also due to their relevance to nuclear materials, space exploration and ion radiotherapy. We have been addressing the stationary states that arise when the projectile follows a periodic trajectory in a solid, by means of a Floquet theory of electronic stopping. A first implementation in a tight-binding setting will be used for illustration, as well as a characterisation of protons shooting across diamond in large-scale time-dependent density-functional theory calculations.

P05

Exploring plasmon properties of the Dirac compound $LiNa_2Bi$ using TDDFT.

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In recent years, 3D topological semimetals (TM)s, which host symmetry-protected 3D Dirac points near the Fermi level, have drawn the attention of researchers in condensed matter due to their vast potential applications [1]. In this study, we investigated the unconventional electronic structure of the recently discovered type-II Dirac compound $LiNa_2Bi$ [2]. Using ab inito time-dependent density functional theory (TDDFT), we studied the plasmon properties of $LiNa_2Bi$. Our analysis goes beyond simple two-band Dirac models that have been often adopted in literature [3,4], since it takes into account the realistic band structure (including the effect of spin orbit coupling) of $LiNa_2Bi$ together with the effects of the electron-electron interaction in the density response function. Our results are crucial for predicting applications of type II Dirac semimetals in optoelectronics.

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P06

Interlayer Excitons in 2D TMD Heterostructures

wo dimensional van der Waals (vdW) heterostructures with several possibilities of band edges alignment are potentially promising candidates in the design of semiconductor junction devices. Moreover, controlling the interlayer excitons in these materials, with highly tunable energies and unique spin-valley physics, lies within the main attempts in quantum information applications based on single exciton and spin. In the present work we predict, based on first principles calculations, a tunable energy shift of the interlayer excitons due to the dipole interaction between the interlayer exciton and the electric field in MoS$_2$/WS$_2$ vdW heterostructure, as a staggered gap semiconductor.

Li vs. Na Solid-State based Batteries : Modelling of Diffusion in Solid Electrolytes

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ABSTRACT

Designing solid-state batteries (SSBs) requires the design of highly efficient solid electrolytes (SSEs) that exhibit high ionic conduction properties. Though they have numerous drawbacks, liquid organic-based electrolytes are the ones most commonly used in the commercial batteries. They are not only dangerous and less efficient but also degrade faster which decreases its life time for long-term applications. Hence the necessity for a safer and longer lived alternative for batteries is a must. To this end, SSEs are now in the forefront of all the materials, as they combine factors of safety (non-flammable), efficiency, lower cost and ease of fabrications. Among them, Doped-LLZO[1] ($Li_7La_3Zr_2O_{12}$) is considered of the most promising ceramics serving this purpose. Herein, we aim to model Li diffusion mechanisms and its respective spectroscopic properties (NMR and EIS[2]) using multi-scale simulations approaches by harnessing both (i) short time and length scales (from DFT and AIMD[3]) and (ii) long time and length scales (from classical MD and KMC[4]) to define multi-scale methodology for understanding the impact of doping have on Li mobility in the material in question by linking the simulations data to the microscopic diffusion measurements (NMR and EIS). Our aim is to develop a Kinetic Monte Carlo model, parameterized with inputs from MD simulations (both classical and *ab-initio*) capable of predicting NMR properties such as ^{7}Li NMR lineshapes and nuclear relaxation times. Density based clustering approaches are employed to analyze Li -trajectories. Additionally, standard DFT-GIPAW calculations are performed for predictions of MAS-NMR[5] spectra of ^{27}Al in Al-doped LLZO (LLAZO). By adapting the same methodology, Na diffusion in NASICON[6] and Sc^{+3} - doped NASICON have been investigated and analyzed.

KEYWORDS: Molecular Dynamics, NMR, DFT-GIPAW, Lithium-diffusion, Solid-State Batteries.

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[1] Lithium Lanthanum Zirconium Oxide
[2] Electrochemical Impedance Spectroscopy
[3] *ab-initio* Molecular Dynamics
[4] Kinetic Monte Carlo
[5] Magic-Angle Spinning Nuclear Magnetic Resonance
[6] **Na** **S**uper **I**onic **CON**ductors

P08 Investigation of the structural complexity of aqueous systems through machine learning

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Studying the microscopic nature of aqueous systems is essential to understanding the underlying laws of macroscopic observations. Thanks to modern machine learning tools, one can now investigate the structural properties in an agnostic way in a high-dimensional space without using only a few pre-defined variables.

I will present two different aqueous systems and show how microscopic structural features can be characterized using modern machine learning tools and graph networks. I will then show that this information can give insights into the underlying physics governing some macroscopic properties of the system.

In the first system, we study the solvation of the 20 amino acids in the water. We show that the cavities hosting these solutes have non-trivial and branchy shapes. Characterizing these shapes by the graph networks, we observe that surprisingly the free energy, enthalpy, and entropy of solvation, can all be predicted using these shapes. We show that for the prediction, one has to consider the branch properties besides the volume and the surface area. It confirms that the model can give all the information needed for the thermodynamics of solvation by looking only at the local density fluctuations of the water molecules.

In the second system, we study the water with surfactant molecules on its surface. Using unsupervised learning tools and machine learning descriptors, we can quantify and cluster the structure of water molecules. We observe three types of local structures, distinguishable at the surface, and show that this information can interpret the SFG results observed in experimental studies, giving an accurate description of the structure through the high-dimensional description and the agnostic unsupervised learning approach.

P09

Development of a computational toolbox to analyse first-passage times and diffusion coefficients in heterogeneous soft-matter systems

The analysis of first-passage time statistics in soft-matter systems, such as water near amino-acid crystals explored in [1], can be vital in understanding the dynamical complexity of their chemical and geometrical properties. From the first-passage time statistics of water molecules, it was shown in [1, 2] that it is possible to infer space-dependent diffusion coefficients in directions normal to various phase boundaries. The analysis developed in [1, 2] is highly nontrivial, computationally expensive, and system dependent. Here, in an inter-disciplinary collaboration between statistical physics and atomistic simulations, we aim to develop a generic computational methodology which will allow us to extract and analyse trajectories, obtained from molecular dynamics simulations by programs such as GROMACS or LAMMPS, to determine first passage times and spatially resolved diffusion coefficients. We performed exhaustive high-performance-computing benchmarks of our algorithm in various aqueous systems, and developed a user-friendly interface that is publicly available for use by active researchers, working on in-silico studies of natural products and other soft matter systems. [1] Roman Belousov, Muhammad Nawaz Qaisrani, Ali Hassanali, and Edgar Roldán. First-passage fingerprints of water diffusion near glutamine surfaces. Soft Matter, 16(40):9202–9216, October 2020. Publisher: The Royal Society of Chemistry. [2] Roman Belousov, Ali Hassanali, and Edgar Roldán. Statistical physics of inhomogeneous transport: Unification of diffusion laws and inference from first-passage statistics. arXiv:2112.08353 [cond-mat], January 2022

P10

Signature of cubic and linear Rashba in $LaAlO_3$ /$KTaO_3$ (0 0 1) heterostructure

P11

Ab-initio characterization of CoTPyP and CoTPyP-Co metalorganic monolayers for catalytic application

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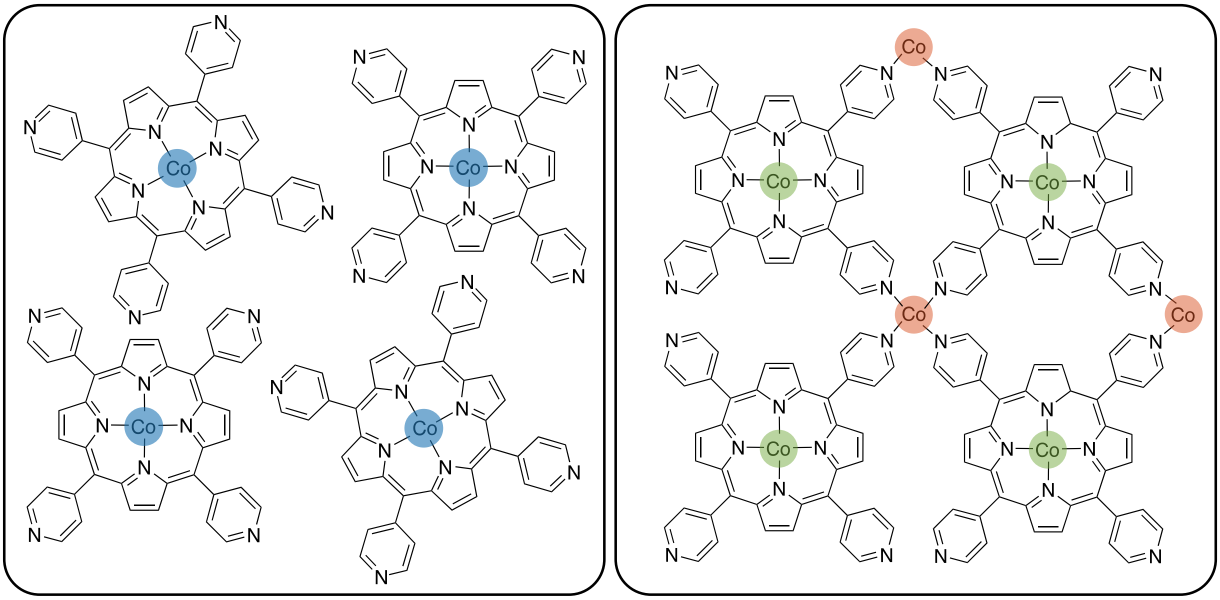
Metalorganic molecules self assembled on surfaces form a template to host regular arrays of metal atoms. Metallic centers act as Single Atom Catalysts (SAC), whose selectivity and efficiency towards specific chemical reactions can be tuned changing either the atomic species or molecular residues, or else the substrate.

Recent experiments have shown the peculiar catalytic activity of a Self Assembled Monolayer (SAM) of TetraPyridyl Porphyrins (TPyP) on an almost free standing graphene sheet. The TPyP SAM has the peculiarity to be able to host two different arrays of SACs, one composed by atoms (M_1) caged in the middle of the porphyrin core and a second one with atoms (M_2) bound to four adjacent molecules, accompanied by a rearrangement of the molecular network.

In order to shed light on its peculiarities, we have extensively investigated this system in different possible configurations within a Density Functional Theory approach. In particular we have characterized a mono- and bi-metaled SAM with Co atoms (M_1TPyP and M_1TPyP-M_2, with M_1,M_2=Co) comparing the results with experimental measurements with different techniques. These calculations firstly helped us to give a better description of the structural changes observed in STM and STS images occurring upon the bi-metalation process. Furthermore, by computing core level shifts, density of states, work function and atomic orbital occupations we could describe the electronic changes occurring in particular at peripherical pyridinic groups (responsible for the binding of the extra Co atoms) and suggest a rationale of the different catalytic selectivity of the central and the peripherical metallic atoms.



P12

Noncollinear relativistic Hubbard parameters and DFT+U with ultrasoft pseudopotentials

Density-functional theory (DFT) has proven to be an extremely successful theory to understand and predict ground state properties of real materials. However, it systematically fails when applied to systems in which the low-energy physics is characterized by localized electrons, for example with d or f character. To remedy this deficiency, Hubbard-augmented DFT functionals (e.g. DFT+U) have been developed in the last 30 years, and successfully applied to the study of weakly correlated oxides. In this work, we extend an implementation of the DFT+U functional in a plane-wave electronic structure code, from a scalar-relativistic to a fully-relativistic pseudopotential (FR-PP) framework. Our formulation is able to deal with FR-PP within the ultrasoft formalism, which allow an efficient plane-wave expansion of the pseudowavefunctions, especially when the electronic charge is heavily localized around the nuclei. We enhance our theory not only with total-energy, forces and stresses calculations, but we also develop a noncollinear linear-response approach based on density-functional perturbation theory, which allow us to evaluate the interaction parameter U from first-principles, in an entirely parameter free scheme.

P13

Automated Many-Body Perturbation Theory

The automation of ab initio simulations is essential in view of performing high-throughput (HT) computational screenings oriented to the discovery of novel materials with desired physical prop- erties. So far, automation has mainly concerned density functional theory (DFT) simulations, and several HT studies were performed with great success. In this work, we propose algorithms and implementations that are relevant to extend this approach beyond DFT, in order to automate many-body perturbation theory (MBPT) calculations. Notably, a novel algorithm pursuing the goal of an efficient and robust convergence procedure for GW and BSE simulations is provided, together with its implementation in a fully automated framework. This is accompanied by an automatic GW band interpolation scheme based on maximally-localized Wannier functions, aiming at a reduction of the computational burden of quasiparticle band structures while preserving high accuracy. The proposed developments are validated on a set of representative semiconductor and metallic systems. Moreover, this automation tools are used to benchmark the Yambo code [1] on the GW100 dataset [2] of 100 molecules, by means of HT automated evaluation of G0W0 ionization potential and electron affinity for all the molecules of the set. For the first time, we provided to the set results obtained within the Godby-Needs plasmon pole model [3] for the dielectric matrix. [1] D. Sangalli et al., J. Phys.:Condens. Matter 31, 325902 (2019). [2] M. J. van Setten et al., JCTC, 11(12):5665–5687 (2015) [3] R. W. Godby and R. J. Needs, Phys. Rev. Lett. 62, 1169 (1989)

P14

Tailoring High-Entropy Oxides (HEOs) as Emerging Radiative Materials for Green Energy Buildings

In the intense research about high-entropy materials and their applications in energy-related technologies, we here discuss the potential applicability of selected oxides and their high entropy alloys in the process of daytime radiative cooling. In particular, by combining density functional and finite difference method we provide an unbiased, scattering-free description of structural, electronic and dynamic features of candidates which show strong radiative properties, mandatory for the best passive cooling performances, while offering the benefits of affordability and compatibility with commercial coating fabrication processes.

P15

The effect of vacancies on the thermoelectric properties of half-Heusler materials

The half-Heusler compound CoTiP with the vacancy-site introduction was investigated in this study. The main goal was to determine the thermoelectric properties affected by the introduction of vacancy, but first, we had to study the electronic properties of these compounds, the results show a change in the nature of the material from an intrinsic semiconductor with indirect band gap to p-type and n-type semiconductor respectively when introducing Co vacancy and Ti, P vacancies, to estimate the thermoelectric efficiency, a ZT value of 0.90, 0.93, and 0.95 was found for Co, Ti, and P vacancy-site respectively. We can deduce from this study that vacancy could improve the thermoelectric (TE) properties of CoTiP half-Heusler, as an augmentation of the Seebeck coefficient is seen, which may be due to the optimized carrier concentration.

P16

Graphitic carbon formation on plasma-exposed polyethylene with molecular dynamics

Here we present an ab-initio modelling of a carbon layer formation on a gas-exposed polyethylene, in the framework of plasma discharges affecting the integrity of polymeric dielectrics in high-voltage cables. Polyethylene (PE) is widely employed in electrical power industry as a low-cost and effective insulator, but undergoes irreversible deterioration associated with partial discharges and the formation of electrical trees. The propagation of such internal defects is self-sustained, and their presence compromise the insulating power and hinders a correct prediction of devices' lifetime. Electrical trees degrade the PE matrix from within, excavating a series of channels in the bulk phase. During the process, the surface conductivity of the channels is enhanced and, as a consequence, the discharge activity is increasingly prevented, producing a misleading scenario for diagnostic detections. Electronic transport on the channels' surface is affected by the chemical evolution of the polymer/gas interface. This involves the formation of a graphite-like structure on the polymer, detected experimentally. No indications are given about the chemical processes involved. In this work, we propose, and validate, a possible mechanism. With molecular dynamics, we reproduced the chemisorption of carbon-rich gaseous molecules on PE, recreating the carbon-bond connectivity in one- and two-dimensions. Geometrical and electronic features of the PE/carbon composites reproduced some hallmarks of graphite structure, suggesting a significant increase in transport properties of PE and recreating a scenario consistent with experimental reports.

P17

First principles characterization of defect states in emerging materials for next-generation technology

The current major worldwide drive for big data, machine learning and quantum computing threatens to overwhelm Si-based resources, which have historically powered information and communication technologies. The search for alternative ones is therefore crucial and it represents a unique opportunity to explore and link materials' properties and performances in unexplored architectures. In this upcoming process, many of the emerging candidates for next-generation technology include disrupting solutions for in-memory computing and synaptic electronics, based on chalcogenides, metal-oxides and other non-Si-based materials in their crystalline, amorphous or disordered phases. Characteristic high densities of defect states play a pivotal role in transport in these systems such that defects and traps practically govern long-term stability and performances of devices. Therefore, describing, identifying, and controlling defect states is crucial to characterize properties of emerging materials and their interplay with non-standard device architectures, as well as to engineer already known materials to improve their application range. I will present some of the work we have been carrying on in such directions within the European projects INTERSECT and OpenModel on different systems. In particular, I will focus on the study of stability, thermodynamics, diffusion, and electronic properties of point defects in crystalline GeSe chalcogenide, a promising material for next generation electronics and photovoltaics. The investigations have been performed by means of the state-of-the-art Quantum ESPRESSO suite of codes and the high-throughput workflows for first principles condensed matter simulations, part of the AiiDA automated infrastructure.

P18

Thermal transport in anharmonic crystals

Recent progress in understanding thermal transport has highlighted how the treatment of anharmonicity can drastically alter prediction on thermal conductivity. This is the case of heat conduction mediated by interband tunneling processes, which emerge between overlapping phonon bands (i.e. with energy differences smaller than their broadenings). This transport channel is enabled by anharmonicity, which broadens the harmonic phonon dispersion, and it is typically neglected in standard formulations, while consisting in the major contribution to thermal conductivity in complex crystals. It is then crucial to describe carefully the anharmonicity in solid state systems in order to quantitatively reproduce transport properties. Here I will report my work about the theoretical framework to properly account for anharmonicity in the calculation of lattice thermal conductivity, with perspectives on how to generalize the formalism beyond perturbation theory.

P19

Plasmonic by design

The manipulation of light on the deep subwavelength scale is essential for enhancing light-matter interactions and improving the performance of nanophotonic devices. For example, the extraordinary properties of hyperbolic metamaterials (HMMs) made them essential for a plethora of applications, ranging from aerospace to automotive, from wireless to medical and IoT. Here, we adopted massive high-throughput computational techniques, based on density functional theory, to design and characterize tunable optical materials that can be used as plasmonic systems in the near-IR and visible range. Starting from simple transition-metal nitrides [1,2], we investigate the role of composition, off-stoichiometry and structural disorder in TiNx compounds [3], and we provide an efficient strategy to fine engineering stable, easy-to-grow HMM superlattices [4,5], with selected optical and extraordinary mechanical properties (e.g. hard materials). Finally, we propose [6] a new class of multifunctional materials, known as high-entropy carbides, that bring together plasmonics, hardness, stability and high temperatures into a single material. These new multifunctional (meta)materials may foster previously unexplored optical/mechanical applications in extreme conditions, e.g. in the fields of aerospace, satellites, and security systems. [1] A. Catellani and A. Calzolari, Phys. Rev. B 95, 115145 (2017). [2] D. Shah, et al., ACS Photonics 5, 2816 (2018). [3] A. Catellani, et al , Phys. Rev. Mater. 4, 015201 (2020). [4] A. Catellani and A. Calzolari, Opt. Mater. Exp. 9, 1459 (2019). [5] A. Calzolari, et al., Adv. Opt. Mater. 9, 2001904 (2021). [6] A. Calzolari et al., Nature Communications, 13, 5993 (2022).

P20

Minimal models for dynamical correlations in transition metal monoxides

Dynamical correlations beyond static mean field theory are of fundamental importance in describing the correlated electronic structure of complex materials, such as transition-metal oxides where the low-energy physics is dominated by interactions between half-filled, very localized d or f shell orbitals. To understand the interplay between screening and localization, high-level and computationally expensive theories - such as DFT+DMFT or GW+EMDFT - are needed. The former addresses local correlations via an effective impurity model with a single self-consistency requirement: namely, that the local Green's function of the lattice become equal to the Green's function of the effective impurity model. The latter extends this approximation to the local part of the polarization function, yielding a comprehensive approach that allows to treat also the effects of long-range interactions. Given the computational complexity of these methods, actual calculations require advanced and expensive numerical implementations and sometimes significantly curtail the number of orbitals to be considered as correlated. Motivated by the success of a recent approach to model local, frequency-dependent correlations in ternary transition-metal oxides via simple frequency-dependent self-energies, in this work we propose a generalization to spin-polarized cases and apply a minimal model to the study of the antiferromagnetic insulating phase of transition-metal monoxides MO (M=Mn,Fe,Co,Ni), considered prototypical materials for beyond-DFT approaches.

P21

High pressure computational search of trivalent di-nitrides

Francesca Menescardi^1, Davide Ceresoli^2 1) DISTAV, Università degli Studi di Genova, Genova, Italy 2) Consiglio Nazionale delle Ricerche, Istituto SCITEC, via Golgi 19, 20133, Milan, Italy Nitrides are much less studied than the corresponding oxides but have been shown to give rise to ultrahard and superconducting materials that can find application in modern technologies as field effect transistors, p-n junctions and energy storage devices. In this work we focus on binary nitrides with a formally trivalent cation, such as a rare-earth ion. These class of compounds are mainly studied in their mononitrate form, which exhibit metallic properties. On the other hand, the corresponding nitrogen-rich pernitrides, that can be synthetized under high pressure, exhibit more intriguing properties compared to the mononitrides. In fact, besides the excellent mechanical properties that arise, when M-N_x compounds are synthesized under pressure, they tend to form fairly long chains of nitrogen atoms. The consequent formation of high energy, single N-N bonds is an effective way to store chemical energy. This is not surprising as nitrogen itself is known to polymerize at 110 GPa and 2000 K, forming the so called cubic gauche structure. Moreover, it is known that the alloying of nitrogen with alkali or with transition metal ions, is an effective way to reduce the polymerization pressure. For these kind of materials, several valence configuration have been proposed to try to explain the nature of the nitrogen bonding. Depending on the valence of the cation, in fact, one can find the pernitride structure, with an oxidation state configuration of M^4+ N_2^4- and an N-N bond length of 1.42 Å (single bond), or a dinitride structure, with an oxidation state configuration of M^2+ N_2^2- and a bond length of 1.23 Å (double bond). The case of a trivalent cation does not seem to fit any of the two definitions, and understanding the nature of nitrogen bonding in this case is not so intuitive. Inspired by a recent work on lanthanum pernitrides, we focused on yttrium dinitride (YN_2) and its formation under pressure. In this work we applied an ab-initio Crystal Structure Prediction method (USPEX) to seek for the most stable YN_2 polymorphs up to 100 GPa of pressure. Then we computed the thermodynamic stability of the obtained structures down to ambient pressure using Quantum Espresso. To understand the nature of the N-N bonding and the oxidation state of these materials, we then compare the obtained results with a set of existing compounds. Besides the observations on the nature of N_2 moieties in the three most stable structures we obtained, we also verified structural and dynamical stability by the means of electronic and phonon DOS.

P22

Phonon anharmonicity at lower mantle conditons: Consequences on the thermal conductivity of MgO

P23

Energies and spectra of correlated metals via the algorithmic inversion of dynamical potentials

Dynamical (frequency-dependent) potentials are needed to predict accurate spectral properties, and arise in embedding theories. The frequency dependence transforms the problem from the diagonalization of an operator (e.g., the Kohn-Sham Hamiltonian of density-functional theory) to the Dyson inversion of a self-energy. Here, we propose a novel treatment of dynamical potentials able to solve Dyson-like equations via an exact mapping to an effective non-interacting problem. The sum-over-poles representation of the self-energy, together with the static contribution to the Hamiltonian, are used to build a (larger) effective Hamiltonian that has the excitation energies of the system as eigenvalues and the Dyson orbitals as a projection of the eigenvectors. The Green's function of the system is also obtained as a sum over poles, and allows for the computation of both spectral and thermodynamic properties. To explore applications on real materials, we introduce a localized-GW Klein functional exploiting the frequency-resolved screened-potential U(ω), and we apply it to calculate the spectral and mechanical properties of SrVO3.

P24

The role of carbon in the formation of α boron during boron carbide synthesis

P25

Looking for metallic states in novel exfoliable 1D materials

One-dimensional materials are extremely attractive due to their unique electronic properties and potential for next-generation applications. A high-throughput screening of experimental inorganic materials has provided a portfolio of more than 800 novel 1D/quasi-1D materials exfoliable from their 3D parent compound, out of which we select a dataset of metallic chains as possible candidates for vias and interconnects. Often, their low-dimensional nature leads to dynamical instabilities in the form of Peierls distortions or charge-density waves (CDW), which drive structural phase transitions. Here, we analyse the stability of these novel materials, identifying the reconstructed stable superstructures from the phonon instabilities. Several interesting behaviors emerge - from Peierls metal-insulator transitions to the emergence of Dirac cone semimetals. In order to get more insight into the mechanisms of the CDW, we investigate the nesting function and the critical role of the electron-phonon coupling, still largely unexplored in realistic quasi-1D systems.

P26

Magnetic properties of octonuclear molecular magnets from first-principles

Molecular nano-magnets are systems of great technological appeal for applications that range from spintronics to quantum information. This work presents a computational study of the magnetic properties of three ring-shaped molecular nano-magnets, each containing eight transition metal atoms: Cr8, V8 and V7Ni. Ab initio calculations, based on Hubbard-corrected non-collinear spin DFT, are used to calculate the effective exchange interactions (including on-site and inter-site anisotropies and Dzyaloshinskii-Moriya couplings) between the magnetic centres, through the sampling of a large number of different spin configurations and a thorough comparison of their energies. The couplings so obtained are then used to construct a generalised Heisenberg Hamiltonian whose diagonalization gives direct access to the ground state of the systems, its low-energy spectrum, its finite-temperature susceptibility and other interesting properties. While the antiferromagnetic ground state of Cr8 is confirmed, the V8 shows an unusual ferromagnetic ground state characterised by a remarkable anisotropy and a high susceptibility to doping which is demonstrated by our preliminary results on V7Ni.

P27

Koopmans spectral functionals: Bridging density-functional and many-body perturbation theory.

Koopmans spectral functionals are able to simultaneously and accurately describe ground state properties and charged excitations of atoms, molecules, nanostructures and periodic crystals. This is achieved by augmenting standard density functionals with simple but physically motivated orbital-density-dependent corrections that enforce the correct description of the charged excitation process. In these formulation state-dependent potentials emerge that can be interpreted as a local and orbital-dependent counterpart to the electronic GW self-energy, albeit already including approximate vertex corrections. We present theoretical evidences supporting this view and numerical simulations showing the excellent agreement with experiments and Green's function methods in predicting charged excitations in a variety of systems ranging from small molecules to crystalline materials. Being this a functional framework,the straightforward advantages are that forces and other derivatives are also readily accessible, and that the numerical parameters are those typical of density functional calculations.

P28

Interplay between structural deformations and flat band phenomenology in twisted bilayer antimonene

In this work we apply first principles calculations to investigate the flat band phenomenology in twisted antimonene bilayer. We show that the relatively strong interlayer interactions which characterize this compound have profound effects in the emergence and properties of the flat bands. Specifically, when the moiré length becomes large enough to create well defined stacking patterns along the structure, out-of-plane displacements take place and are stabilized in the regions dominated by the AB stacking, leading to the emergence of flat bands. The interplay between structural and electronic properties allows for detection of flat bands in higher twist angles comparable to other two-dimensional materials. We also show that their energy position may be modulated by noncovalent functionalization with electron acceptor molecules.

P29

Strain-tronics: a mechanical way to control 2D materials

Discovery of graphene created a now large scientific community working on the properties of 2D materials. A branch in the field that is now acquiring increasing attention is the ability of apply mechanical deformation to the 2D materials and their ability of sustain larger strain with respect their bulk counterpart. Indeed, it has been proven one can apply strain to a layered materials in a more reproducible way than in bulk. Moreover, the materials respond strongly to the external deformation. This observation paves the way to controlling the response of a 2D material through mechanical methods. In this talk, I will introduce some of the recent results in the field and compare with some experimental evidence. A careful ab-initio investigation is able to provide a in-depth physical description of the phenomenon.

P30

Magnetic Transparent Conductors

Transparent Conductors (TCs) represent a class of materials that have attracted much attention because of the peculiar interplay between optical and transport properties and thanks to potential applications, for example in solar energy devices. The most common and investigated TCs are n-doped oxides: the search for potential non-oxides TCs can deepen the basic understanding of such a class of materials and enlarge the functionalities of TCs including magnetic effects, that have been so far investigated only in few cases considering oxides compounds where the transparency of the material is affected by growth conditions, emergence of mid-gap states, oxigen vacancies and other environmental conditions. By using High-Throughput screening techniques we have filtered 115 TCs and identified among them few non-oxides compounds that exhibit a finite magnetization when doped with transition-metals, becoming magnetic-TCs.

P31

Sn deposited on Ag(001): A question of size

We have investigated the evolution of the structure and electronic properties of Sn deposited on the Ag(001) surface. We have performed density functional theory calculations, together with low energy electron diffraction (LEED) and angle-resolved photoemission spectroscopy (ARPES) experiments. We find the somewhat surprising result that for all coverages of Sn up to 1 ML, Sn-Ag bimetallic substitutional surface alloys are thermodynamically favored. The unit cell and structural configuration changes with Sn coverage. In the bulk, Sn and Ag atoms have almost the same size. However, interestingly, though the effective size of surface Ag atoms is less than that of bulk Ag atoms, the effective size of the Sn atoms is bigger than that of bulk Sn atoms, as well as both surface and bulk Ag atoms. As a result, the formation of a Sn-Ag surface alloy relieves tensile surface stress. Theoretically computed band dispersions for substitutional surface alloy models agree well with the experimentally observed ARPES data.

P32

Phase transition of Dion-Jacobson Perovskites

We present an ab-initio study performed by means of Density Functional Theory (DFT), more specifically by computing the hyperfine parameters, to direct the design of Dion-Jacobson perovskite systems with novel properties and therefore aid experimental synthesis. From this study it is possible to obtain information regarding the structural properties and local landscapes, such as octahedra rotations, tilts and distortions which occur during a structural phase transition, and that will aid and complement the interpretation of analysis performed through Perturbed Angular Correlation (PAC) radioactive nuclear techniques. We focus our study on the CsNdNb2O7 system characterized by a high-temperature P4/mmm (S.G. 123) centrosymmetric structure and a ground-state P21am (S. G. 26) ferroelectric system. We have probed potential candidates that may form the pathway transition through the P4/mmm -> P21am structural phase transition; this phase has been identified as being the C2/m (S.G. 12) structure. The three phases were then analyzed to probe the electronic properties (band gap widths and partial density of states; PdoS) and electric field gradients. Since the Nd possess strongly localized and partially filled f-states, we were required to resort to DFT+U, were U refers to the effective Hubbard potential. By probing the PDoS we observe a direct relation regarding the tilts and rotations of the O perovskite cages as the transition occurs; these show some variations mostly for the O p-states which contribute mostly to the valence band maximum and consistent with the distortions from the high-symmetry to the low-symmetry phase.

P33

Designing Energy Materials Using Carbon Allotropies

This talk aims to explore the promising applications of several carbon allotropies such as twin-graphene and its structural derivatives and a newly proposed allotrope named pentagraphyne in the field of energy and electronics as well. These allotropies have an intrinsic band gap and are suitable for many technological applications. Using density functional theory methodology, structural and electronic properties of these materials will be discussed with special emphasis on nanoscale capacitor and anode-material designing. Twin-graphene immerged as an excellent candidate for optoelectronics, nanocapacitor and Na/Mg-ion batteries. Next, we have investigated the structural, mechanical, electronic and optical properties of novel two-dimensional carbon material, namely pentagraphyne which is energetically favourable than other graphyne members. Remarkable carrier mobility along with its superior optical performance renders it to be a potential candidate for future electronics, photovoltaic solar cells, and optoelectronic devices. Pentgraphyne also shows potential as an anode material for designing Li/Na ion batteries. References: 1. J. Deb, D. Paul, U. Sarkar, J. Mater. Chem. C 2020, 8, 16143-16150. 2. J. Deb, U. Sarkar, Applied Surface Science 2021, 541, 148657. 3. J. Deb, H. Dua, U. Sarkar, Phys. Chem. Chem. Phys. 2021, 23, 16268–16276. 4. H. Dua, J. Deb, D. Paul, U. Sarkar, ACS Appl. Nano Mater. 2021, 4, 4912-4918. 5. J. Deb, R. Ahuja, U. Sarkar, ACS Appl. Nano Mater. 2022, 5, 10572–10582. 6. H. Dua, J. Deb, U. Sarkar, Energy Storage 2022. https://doi.org/10.1002/est2.371

Evolution of Structural, Magnetic and Electronic Properties with Pressure in TMPX_3 van-der-Waals Compounds

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Control of dimensionality in condensed matter continues to reveal novel quantum phenomena and effects. $TMPX_3$ (e.g. $FePS_3$) have proven to be ideal examples where structural, magnetic and electronic properties evolve into novel states when their dimensionality is tuned with pressure. At ambient pressure, they are two-dimensional van-der-Waals antiferromagnets, and Mott or charge-transfer insulators. Our recent studies [1-4] have reported dimensionality crossover related pressure-induced insulator-to-metal transitions and novel magnetic phases. There are also reports of superconductivity in a related member of this family of compounds [5]. To further understand the structure and physical property evolution with pressure, we have performed a random structure search using first-principles calculations at high pressures and DFT+U studies to elucidate relationship between structural transitions, magnetism and electronic properties. Our computational explorations into the pressure-tuned $TMPX_3$ are expected to guide the discovery of novel phases and superconductivity in these van-der-Waals systems. This work has been available on cond-mat.str-el, arXiv:2209.05353 (2022)

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P35

Crossover from Peierls-Boltzmann to Wigner thermal transport in thermoelectric skutterudites

Skutterudites are crystals with a cage-like structure that can be filled with rattling atoms, usually leading to a reduction in thermal conductivity that can be exploited for thermoelectric applications. Here, we leverage on the recently introduced Wigner formulation of thermal transport to elucidate the microscopic physics underlying heat conduction in skutterudites, showing that filler atoms can drive a crossover from the Boltzmann to the Wigner regimes of thermal transport, i.e. from particle-like conduction to wave-like tunnelling. At temperatures where the thermoelectric efficiency of skutterudites is largest, wave-like tunneling can become comparable to particle-like diffusion. We define a Boltzmann deviation descriptor able to differentiate the two regimes and relate the competition between the two mechanisms to the materials' chemistry, providing a design strategy to select optimal rattlers and identify optimal compositions for thermoelectric applications.

P36

Information content in liquid water: from bulk to hydrophobic surfaces

Hydrophobic surfaces are ubiquitous in nature and play an integral part of chemical or biological systems. Despite it’s importance, understanding the structure of hydrophobic surfaces remains an open challenge. The air-water interface is one of the most prototypical hydrophobic surfaces that has been studied from both experimental and theoretical fronts. In this work, state-of-the- art information theoretical techniques are used to characterize the correlations in the hydrogen bond network in the bulk and at the surface of water obtained from atomistic simulations. Using a synergy of both machine learning inspired local atomic descriptors as well as chemical intuition based parameters, we elucidate which combinations of variables are most suited to describe the high-dimensional fluctuations in water. In this regard, we elucidate the challenges in using single variables in characterizing local environments in the bulk. Information theory provides a unique perspective on understanding the microscopic origins of surface-tension and further opening new directions in information flow for understanding non-equilibrium phenomena in aqueous systems.

P37

Comparative study of the fundamental properties of Ga2O3 polymorphs

Full potential linearized augmented plane wave method plus local orbitals (FP-LAPW+lo) on the basis of Density Functional Theory (DFT) is called to study the structural, electronic, elastic, optical, thermodynamic and transport properties of four different phases of Ga2O3 denoted by α, β, δ, and ε. The calculated gap energy Eg for the stable polymorph β-Ga2O3 using the modified Becke-Johnson (mBJ) exchange potential is 4.6 eV which lies in the deep ultraviolet range making Ga2O3 promising for optoelectronics. Thermal effects on some macroscopic properties such as heat capacity, thermal expansion coefficient, Grüneisen parameter and Debye temperature are predicted using the quasi-harmonic Debye model. The analysis of transport properties for β-Ga2O3 using semi-classical Boltzmann transport theory in temperature range between 300 and 1000 K showed high Seebeck coefficient S=-348.4 µVK-1 at room temperature with huge power factor PF= 39.5×1010 WK-2m-1s-1 at T=1000 K. This suggests that Ga2O3 is a potential thermoelectric material.

P38

Single k-point spin Chern number in a supercell framework for disordered two-dimensional topological insulators

We present an approach for the calculation of topological invariant in disordered two-dimensional quantum spin Hall insulators. Standard methods are based on the knowledge of eigenstates of defined momentum k and their evolution throughout the Brillouin zone. The introduction of disorder breaks the translational symmetry and implies the use of large simulation cells, where the k-point sampling is typically reduced to the single Gamma point. Here, we introduce a single-point formula for the spin Chern number that enables to study disordered quantum spin Hall insulators within the supercell framework. Inspired by the work of Prodan [1], our approach allows to calculate the spin Chern number even when the spin Sz is not a good quantum number. We validate our method on the Kane-Mele model, both pristine and disordered, and study the robustness of the quantum spin Hall phase with respect to Anderson disorder. Finally, we investigate the disorder-driven transition from a trivial to a topological phase known as topological Anderson insulator. [1] E. Prodan, “Robustness of the spin-Chern number”, Phys. Rev. B 80, 125327 (2009).

P39

Two-Dimensional Silicene–Stanene Heterostructures by Epitaxy

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The synthesis of new Xenes and their potential applications prototypes have achieved significant milestones so far. However, to date the realization of Xene heterostructures in analogy with the well known van der Waals heterostructures remains an unresolved issue. Here, a Xene heterostructure concept based on the epitaxial combination of silicene and stanene on Ag(111) is introduced, and how one Xene layer enables another Xene layer of a different nature to grow on top is demonstrated. Single-phase (4 × 4) silicene is synthesized using stanene as a template, and stanene is grown on top of silicene on the other way around. In both heterostructures, in situ and ex situ probes confirm layer-by-layer growth without intercalations and intermixing. Modeling via density functional theory shows that the atomic layers in the heterostructures are strongly interacting, and hexagonal symmetry conservation in each individual layer is sequence selective. The results provide a substantial step toward currently missing Xene heterostructures and may inspire new paths for atomic-scale materials engineering. [1]

[1] Daya Sagar Dhungana et al., Adv. Funct. Mater. 2021, 31, 2102797

P40

Ab initio study of many-body non-linear optical response tensors

We present a theoretical and computational scheme for calculating the many-body interacting second-order optical response to light from first principles. Our practical implementation starts from the length-gauge formulation of the non-interacting second-order optical response in semiconductors [1] based on localized Wannier functions [2] and pursues within the time-dependent current-density functional theory framework in order to take into account many-body interactions and extract the interacting quadratic optical response [3]. We incorporate metallic terms within the non-interacting formulation by retaining occupation derivative terms and in this way we extend our scheme also to metals. It is also worth noting the use of a time-dependent response theory based on the current-density instead of the density in order to preserve the explicit tensorial character of the response and boost a natural connection with the independent-particle picture in the optical limit and, by extension, with the Wannier-interpolation shceme. The outcome allows us to analyze in detail the impact of many-body interactions on second-order photocurrents as well as discuss the interplay of linear responses at subsequent orders. Funding provided by the European Union's Horizon 2020 research and innovation programme under the European Research Council (ERC) grant agreement No 946629. [1] J. E. Sipe and A. I. Shkrebtii, Phys. Rev. B 61, 5337 (2000). [2] J. Ibañez-Azpiroz, S. S. Tsirkin and I. Souza, Phys. Rev. B 97, 245143 (2018) [3] E. Luppi, H. Hübener and V. Véniard, Phys. Rev. B 82, 235201 (2010)

P41

Emergent controllable topological phases in van der Waals heterostructures

Despite the huge expansion in the family of 2D materials, quantum spin Hall and Chern insulators have remained rare and elusive, with most monolayers displaying topologically trivial properties. Still, combining such trivial 2D materials into van der Waals heterostructures offers combinatorially vast opportunities to realise emergent topological order. Here, not only we disclose different strategies to engineer topological heterostructures out of trivial insulating layers, but we also show how the emergent topological phase can be controlled by external means. On one side we report on the possibility to switch the Chern number of a heterostructure by varying the magnetization orientation through an external magnetic field. On the other, we propose to achieve a non-volatile electric-field control of a quantum spin Hall phase by combining a ferroelectric monolayer with a trivial 2D insulator. All theoretical scenarios are validated through accurate first-principles simulations and by screening 2D databases for realistic materials platforms.

P42

Thermodynamics and Dielectric Response of BaTiO3 from an integrated machine learning model

Modeling the ferroelectric transition of any given material requires three key ingredients: (1) a model of the potential energy surface, that describes the energetic response to a structural distortion; (2) the free energy surface sampled at the relevant, finite-temperature conditions; and; (3) the polarization of individual configurations that determines, through averaging over samples, the observed polarization and the phase transitions. To this aim, we make use of an integrated machine-learning framework, based on a combination of an interatomic potential and a vector model for microscopic polarization, which we use to run Molecular Dynamics simulations of ferroelectrics with the same accuracy of the underlying DFT method, on time and length scales that are not accessible to direct ab-initio modeling. This allows us to uncover the microscopic nature of the ferroelectric transition in barium titanate (BaTiO3). The presence of an order-disorder transition is the main driver of ferroelectricity, while the coupling between symmetry breaking and cell distortions determines the presence of partly-ordered (tetragonal and orthorhombic) phases. The framework also allows us to reconstruct the temperature-dependent BaTiO3 phase diagram, with first-of-its-kind accuracy. Finally, we compute the frequency-dependent dielectric response function, finding a dielectric response profile qualitatively similar that obtained with previous effective-Hamiltonian simulations as well as to experimentally measured profiles, with some remaining discrepancies that we trace back to the underlying DFT functional. We expect this integrated, generally applicable modeling technique to become a valuable tool for elucidating the ferroelectric behavior of a wide variety of materials.

The effect of metal electrodes on transport properties of transition metal dichalcogenides

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Silicon (Si)-based FET, highly employed in our life, face several issues like large off-state leakage current and high-power consumption especially when they are scaled down to sizes less than10 nm [1, 2]. Therefore, scientists have been looking for new materials which are able to improve devices' electronics while replacing silicon semiconductors in device manufacturing. Transition Metal Dichalcogenides (TMDs) are among the promising candidates since they have both high carrier mobility and sizable gaps [3,4]. In this study, we investigate the effect of Two-Dimensional (2D) metal electrodes on the transport properties of several lateral heterostructures (LH) (metal/semiconductor pairs) which could allow developing efficient electronic devices below the micrometer size. We consider differences in work function and strain between the interface's components crucial factors for developing new 2D devices. We find that, apart from the mentioned factors, open d-shell plays a critical role in the electron transmission of the materials.

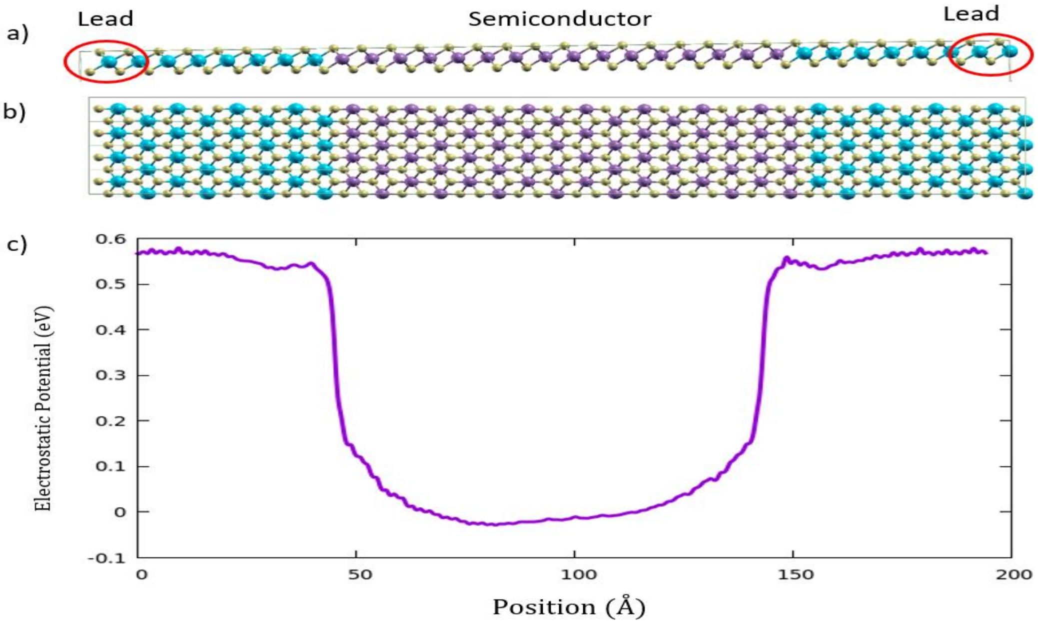

Figure 1: a) side view, b) top view, and c) Electrostatic potential of scattering region

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A comparison of LDA, PBE, and PBEsol on high temperature and high pressure thermodynamic properties of metals: the case of molybdenum and tungsten.

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We compare the PBEsol functional (Perdew et al., Phys. Rev. Lett. **100**, 136406 (2008)) with the local density approximation (LDA) and the PBE (Perdew et al. Phys. Rev. Lett. **77**, 3865 (1996)) generalized gradient approximation for the calculation of the thermodynamic properties of body-centered cubic tungsten and molybdenum, refractory metals that have attracted a lot of interests for their high melting point and corrosion resistance. The three functionals are compared on the phonon dispersions, the temperature dependent thermal expansion, isobaric heat capacity, adiabatic bulk modulus, and average Grüneisen parameter, at zero and finite pressures, and on the thermal pressure-volume equations of state. [1] At zero pressure we compare our results with experiments, while at high pressure we compare with empirical models based on fits of the equations of state and of low pressure experimental data. In some cases, we compare also with previous ab-initio calculations.

[1] Automatic work-flows for the calculation of these quantities within the quasiharmonic approximation are implemented in the `thermo_pw` package.
See `https://dalcorso.github.io/thermo_pw/`.

P45

Predicting hot-electron free energies from ground-state data

Machine-learning interatomic potentials, while extremely successful in describing condensed phases, are usually trained on ground-state electronic-structure calculations depending exclusively on the atomic positions and ignoring the electronic temperature. Hence, they are limited in their ability to describe thermally excited electrons. We introduce a rigorous framework to calculate the finite-temperature electron free energy based exclusively on ground-state total energy and electronic density of states, while allowing to sample on-the-fly the electronic free energy at any temperature. Our physically-motivated approach facilitates modelling material properties at extreme conditions with a fraction of the usual cost. We demonstrate it by computing the equation of state and heat capacity of metallic hydrogen at planetary conditions. This approach demonstrates the impact of a universal model describing structural and electronic properties inexpensively and its ability to enable more accurate and predictive materials modelling and design. Reference: Chiheb Ben Mahmoud, Federico Grasselli, and Michele Ceriotti, "Predicting hot-electron free energies from ground-state data", Phys. Rev. B 106, L121116 (2022)

P46

Many-body effects in finite momentum transfer electron energy loss spectroscopy of freestanding graphene

In this work, we unravel the importance of many-body effects on the finite momentum EELS (electron energy loss spectrum) of freestanding graphene by comparing very recent experimental data obtained with high resolution in energy and momentum with ab initio calculations. Calculations are performed at increasing levels of theory, elucidating the importance of the electron-electron (e-e) interaction in the quasi-particle properties (included with the GW method) and the electron-hole (e-h) interaction (included by solving the Bethe-Salpeter equation). Both interactions need to be included in the description of the EELS to obtain a quantitative agreement with experiments, and we observe that while the excitation gap dispersion is dominated by e-e interaction, the dispersion of the π plasmon is governed by an expected constant e-e and an unexpected e-h interaction increasing with momentum transfer. Both the shapes of the onset and the π plasmon are significantly affected by the e-h effects.

P47

Novel Materials for Emerging Sustainable Energy Storage: Rechargeable Lithium- and Sodium-ion batteries

The development and optimization of novel energy storage materials are accelerated by computational design and analysis. Lithium and sodium-ion rechargeable battery electrodes have relied on intercalation compounds, which allow metal ions to incorporate into a host structure without significantly altering the structure. Using density functional theory (DFT) with (out) Hubbard correction (DFT+U), ab initio molecular dynamics simulations, and a tight-binding model to benchmark A2MnSiO4 (A = Li, Na) cathode materials for Alkali-ion batteries at bulk phase, surface, and cathode/electrolyte interfaces, charge-transport mechanisms and their modification strategies will be discussed.

P48

Ab Initio Maximally-Localized Exciton Wannier Functions for Solids

Since their introduction nearly 25 years ago, maximally-localized Wannier functions (MLWFs) have had a transformative impact on our ability to compute and understand one-electron observables using density functional theory (DFT). Today MLWFs, serve as a compact basis for linear scaling algorithms, allow for the computation of Berry phase (geometric) quantities (e.g. polarization in electronic structure theory), and find application in efficient and accurate interpolation of linear response quantities (e.g. electron-phonon matrix element), and more. However, to date the MLWF framework has been applied to single-particle excitations. Excitons, correlated electron-hole pairs, dominate the optical response in gapped materials and understanding these composite particles plays an important role in the design of next-generation optoelectronic devices. Here, we leverage the MLWF scheme to construct maximally localized exciton Wannier functions (MLXWFs), representations of two-particle electron-hole states where the gauge freedom is used to enforce localization in the average electron-hole coordinate. As a proof-of-concept, we apply our framework to low-lying singlet and triplet excitons, computed with the ab initio GW plus Bethe-Salpeter approach, in the ionic solid LiF. We plot the MLXWFs, detail the convergence of their spreads, and show how a Wannier-Fourier interpolation scheme can be used to efficiently interpolate the exciton dispersion throughout the Brillouin zone. Our work paves the way towards the ab initio construction of exciton tight binding models, efficient interpolation of the exciton-phonon vertices, computation of the Berry-curvature for exciton bands, and more.

P49

Hubbard interactions in magnetic monolayers: FePS$_3$ and CrI$_3$

Hubbard-corrected density-functional theory has proven to be successful in addressing self-interaction errors in 3D magnetic materials. However, the effectiveness of this approach for 2D magnetic materials has been much less explored. Here, we use PBEsol+U and its extensions PBEsol+U+V to investigate the electronic, structural, and vibrational properties of 2D antiferromagnetic FePS$_3$ and ferromagnetic CrI$_3$. The Hubbard parameters (onsite U and intersite V) are computed self-consistently using density-functional perturbation theory (DFPT) [PRB 98, 085127 (2018)], thus fully from first-principles. We show that for FePS$_3$ Hubbard corrections are crucial for obtaining the experimentally observed insulating state with the correct crystal symmetry, with Hubbard-corrected vibrational frequencies in good agreement with Raman experiments. Finally, we discuss CrI$_3$, and the requirements it elicits in correcting the relative positions of the majority and minority conduction bands via a spin-resolved U [PRB 98, 235157 (2018)].

P50

Control of the exchange coupling in graphene-based synthetic antiferromagnets

The search for efficient and new synthetic antiferromagnets has intensified in the last few years. Synthetic antiferromagnets have weaker coupling than the crystal ones and allow for easier manipulation. Furthermore, their magnetic texture can be probed by conventional techniques used for ferromagnets, which gives them a significant advantage over crystal ferromagnets (Duine et al, Nat. Phys. 14, 217, 2018). Using graphene as a spacer towards creation of synthetic antiferromagnets has been proven to be a successful approach (Gargiani et al, Nat. Commun. 8 ,699, 2017). The existing Fe/graphene/Co synthetic antiferromagnets are very promising and have been created experimentally. Ability to tune their exchange coupling and potentially to switch them to the ferromagnetic state in a controlled manner would bring new functionalities. The goal of this work is to model the surface for the system of Fe/Gr/Co in order to confirm the AFM and FM couplings viewed in experiment, before and after the beam irradiation. In collaboration with the experimental groups from Elettra, Trieste, we aim to understand the microscopic mechanisms behind the switching of the magnetic coupling. The main method used for this goal is the first principles Density Functional Theory calculations.

Effect of Ni and CeO2 surfaces on dry methane reforming

Climate crisis and alarmingly high rates of atmospheric CO2 emissions have prompted researchers to look for novel ways of CO2 capture, removal and utilization. Very high stability of the CO2 molecule, which requires about 530 kJ/mol for the C=O bond to dissociate, presents a challenge in its utilization. On the other hand, methane is an abundant hydrocarbon source with an even higher global warming potential. One of the promising ways for large-scale methane and CO2 utilization is dry reforming of methane, where CO2 and CH4 are converted into syngas (H2 and CO). Nickel-decorated CeO2 nanorods, nanocubes and nanospheres are promising catalysts, which exhibit high turnover frequencies and great selectivity. Therefore, we investigated experimentally and theoretically the structure and performance of these catalysts. Extensive quantum chemistry calculations were performed to explain the experimental observations. Ceria can exhibit different facets with various terminations, depending on the method of synthesis and chemical potential of oxygen. Using DFT, different ceria surfaces (111, 110 and 100) were studied with different surface terminations. CO2 adsorption was modelled on these surfaces and three distinct adsorption modes were discovered (monodentate, bidentate, carbonate), which is consistent with experimental observations (TPD-CO2). Adsorption energies vary from 0.2 eV for weak monodentate binding to over 1.5 eV for strong carbonate formation. Activation of CH4 over nickel nanoparticles was also modelled. On extended Ni(111) and Ni(100) surfaces, the activation barrier was found to be 0.71 eV and 0.54 eV. Variously sized icosahedra, octahedra, truncated octahedra and cubes were investigated and found to exhibit lower activation barriers and, thus, higher activities. Cubes are most active because they exhibit (100) surfaces but are also least stable. Truncated octahedral are active on the truncated surfaces, where (100) is present. Icosahedra and octahedral are less active and lose activity as their size increases. Published: K. Lorber, J. Zavašnik, I. Arčno, M. Huš, J. Teržan, B. Likozar, P. Djinović. CO2 activation over nanoshaped CeO2 decorated with nickel for low-temperature methane dry reforming. ACS Appl. Mater. Interfaces 2022, 14, 28, 31862–31878

P52

First-principles calculation of anomalous Hall and Nernst conductivity by local Berry phase

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We have implemented a finite-difference algorithm for computing anomalous Hall and Nernst conductivity in OpenMX, a software package for nano-scale material simulations based on density functional theory [1,2]. We extended the methods to a metallic system based on the expression to evaluate the Berry curvature in an insulating system [3]. We calculated anomalous Hall conductivity and Nernst conductivity in a two-dimensional ferromagnetic material $FeCl_2$ and three-dimensional ferromagnetic transition metals bcc-Fe, hcp-Co, and fcc-Ni. Our results are comparable to previously reported results computed by Kubo-formula or Wannier representation. The detailed Fermi-energy dependence of the anomalous Hall conductivity is required to evaluate anomalous Nernst coefficients. Since our implementation requires only once-shot computation for the overlap matrix of the periodic part of Bloch wave functions to evaluate anomalous Hall conductivity for multiple Fermi energies, the calculations are very efficient, and the anomalous Nernst coefficients can be calculated faster than other implementations. The present method will open an efficient material design of transverse-thermoelectric materials.

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DFT study of the influence of short-range C–C pair interactions on C diffusion in α-Fe (bcc)

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Many important phenomena, such as material ageing, involve impurity diffusion in solids [1]. Diffusion of small chemical elements (H, B, C, N and O) in metals typically occurs via an interstitial mechanism [2]. Among small elements, carbon occupies an essential role in iron alloys as it is the most effective addition to martensitic steel. This steel possesses a large number of industrial and technological applications related to its higher strength compared to other materials [3]. The presence of neighboring impurities modifies significantly the diffusion process. Indeed, it is impossible to study these short-range impurity interactions by experimental techniques and theoretical studies are the only way to understand correctly the influence of these interactions on the diffusion properties atomic level.

We studied in detail the C diffusion in presence of other carbon atoms by DFT (with VASP code) and KMC techniques. We studied all possible C-C pair configuration corresponding to energy local minima with C-C distances up to 6Å. Using the NEB technique [4], we found all migration paths with saddle points between these local minima (Fig1 a/b). This *first principle* energy database was introduced in kinetic Monte Carlo simulations to compute the thermodynamic and kinetic parameters.

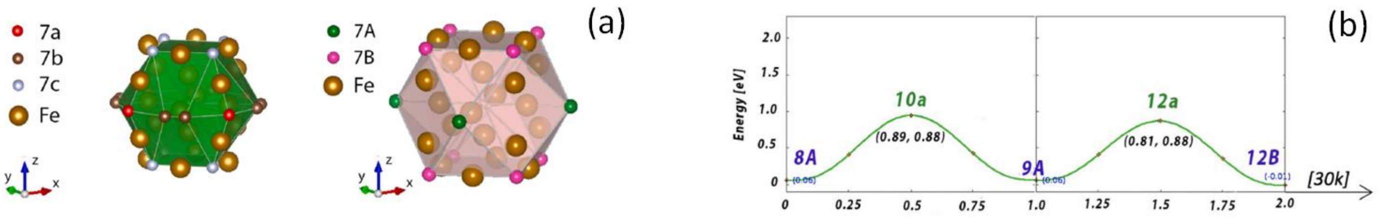

Figure 1. Stable C-C configurations (a) are used to find migration saddle points during diffusion (b).

According to our simulations, C–C pair repulsive interactions lead to (1) the modification of the order/disorder transition conditions depending on the carbon content and temperature; (2) the increase of the carbon diffusivity, especially along the Zener ordering direction (up to ten times); (3) the important kinetic correlations. These results show that diffusion coefficient D_x slightly depends on C–C interactions (at 4 at.% C, D_x is about 10% higher when C–C interactions are included). On the other hand, diffusion coefficient D_z highly depends on C–C interactions (at 4 at.%C, D_z is one order of magnitude higher when C–C interactions are taken into account) [5].

These effects should be taken into account for an accurate prediction of low-temperature ageing in ferritic and martensitic Fe–C alloys.

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P54

Electronic properties of BaTiO3/metal oxide interfaces

Barium titanate is a widely known and studied perovskite material. In its tetragonal phase, it exhibits ferroelectricity due to inversion symmetry breaking during cubic-tetragonal phase transition. Coupling ferroelectricity with ferromagnetism can lead to new opportunities in the electronic device industry, which lead to studies where barium titanate is combined in different heterostructures. In this work, we are investigating electronic properties at the BaTiO3/metal oxide interfaces. Prior to electronic properties investigation, 3 different heterostructures comprising of different metal oxides coupled with barium titanate are relaxed, and the structural changes at the interface are analysed. A number of physical quantities that give us information about the charge mobility at the interface are also investigated, including charge carrier effective mass, electrostatic potential across the heterostructure, and charge density. Looking into the charge mobility at the interface can give us crucial information on potential use of studied materials in optoelectronic devices, as well as their potential use in other electronic devices.

P55

Strain-induced topological phase with high mobility and low lattice thermal conductivity

Topological insulators having edge states which are becoming hope to provides ground for lossless carrier transport when used as channel material in a transistor. On considering it we have studied hexagonal antimonene monolayer with 15% tensile strain to reach topological phase and employed electron phonon coupling through EPW code and predicted electron and hole mobilities in Sb system as a function of temperature. Comparing with the pristine or without strain we found 1 order magnitude increase in mobilities. With this we explored the lattice thermal conductivity and found a huge reduction >60 % in the 15% phase compare to the 0%. These properties give it flavor of possible thermoelectric as well.

A combined G_0W_0/BSE scheme of characterizing surface polaron photoexcitations in hydroxylated rutile $TiO_2(110)$

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In reduced TiO_2, electronic transitions originating from polaronic excess electrons in surface-localized band-gap states (BGS) are known to contribute to the photoabsorption and to the photocatalytic response of TiO_2 in the visible region. Recent state selective studies using two-photon photoemission (2PPE) spectroscopy have also identified an alternative photoexcitation mechanism contributing to the photoabsorption of the reduced surface (110) of rutile TiO_2. This process involves *d*-*d* excitations from BGS arising from surface and subsurface defects, including bridging hydroxyls and oxygen vacancies[1–3]. Density Functional Theory (DFT) has been used to determine the character of the electronic excited states involved in a $d_{t_{2g}}$-$d_{t_{2g}}$ transitions[1, 2], but its accuracy is questioned by its theoretical framework: DFT is in principle exact for ground state systems and does not describe interacting photogenerated electron-hole pairs, i.e. the excitons. This has highlighted the need to move beyond the DFT formalism, by working within a many-body perturbation theory (MBPT) framework where excitations are described as a collection of effective particles propagating through the system. In this poster I will show how a G_0W_0 method combined with the solution of the Bethe-Salpeter equation (BSE) provides a powerful tool for characterizing from first principles the optical excitations from BGS as identified by 2PPE experiments on hydroxylated $TiO_2(110)$.

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P57

Machine Learning Interatomic Potential approach for diboride under different temperature: Take TiB2 as an example

The discovery of new materials with outstanding property combinations as well as advancing the performance of materials in use—to ultimately optimise their sustainability and biocompatibility—is the main quest of modern technologies. Well established in both scientific as well as industrial context, TMBs are valued for their high chemical and thermal stability, incompressibility and excellent high-temperature strengths, high melting points, corrosion resistance, as well as electrical and thermal conductivity. But the applicability of TMBs, however, is severely limited by their brittleness. I would like to showcase how the problem of costly and “small”-scale quantum-mechanical simulations can be overcome by developing machine learning interatomic potentials. These allow for computational efficiency without losing accuracy and insight in the electronic structure. Employing the potentials, it will develop for modelling mechanical deformation at various temperatures with the aim to provide atomic-level understanding of strengthening/toughening mechanisms and derive design guidelines for their targeted modifications.

P58

Phase diagram of iron in Earth's core from deep learning

Iron is considered to be the main component of Earth's core. Substantial efforts have been made to understand its phase diagram and physical properties at extreme conditions. However, it remains debated about how the atoms in solid iron are arranged at Earth's core conditions, where possible candidates include hexagonal close-packed (hcp), body-centered cubic (bcc), and face-centered cubic (fcc) structures. As crystal structure and physical properties are closely related, there is also a significant uncertainty in the properties of Earth's core, such as elasticity, heat conductivity, and density, making the accurate interpretation of seismic observations difficult. Here we aim to study the phase stability of solid iron at Earth's core conditions. For this, a deep-learning interatomic potential was developed with ab initio accuracy but is more cost-effective. We then directly compute the free energy of the bcc, fcc, and hcp phases by performing large-scale molecular dynamics simulations. The calculated free energy allows for determining the phase stability of solid iron in Earth's core.

P59

Sensing capabilities of ultrathin BaTiO3 nanostructures toward carbon oxides based on optical signals

Due to the large presence of carbon oxide gases in both our environment and industry, there is an ongoing search for simple and efficient gas sensors. As a response to the current challenges toward lower limits of detection, in this work we propose a detection of optical signals from ultrathin BaTiO3 nanostructures as the basis for carbon oxides sensing. Based on density functional theory, we simulate the sensitivity of electrical and optical properties of the ultrathin BaTiO3 nanostructure with respect to different adsorption sites on the (001)-BaTiO3 surface. Significant changes in the optical activity, including absorption, reflection and EELS spectra, are detected. Supercell model study showed that optical signals follow a monotonous trend with respect to the molecule concentration. The changes are explained via charge transfer between the (001)-BaTiO3 surface and the adsorbed gas molecules. An insight into the physical and chemical nature of the processes at the nano-scale improves our understanding of the sensing mechanism. At the same time, the obtained results might pave a way to new easy-to-use but robust sensor designs.

DFT study of electrooxidation catechol mechanism in water solution on Pt-electrode

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We have optimized and calculated the IR absorption spectra of pyrocatechol, o-benzoquinone, and intermediate reactants based on DFT using hybrid functionality B3LYP on the basis of 6-31G(d). The calculation was carried out taking into account the influence of the medium within the framework of the polarized continuum model, which we tested earlier [1-2] and it corresponds to the experimental conditions of the electrochemical oxidation of pyrocatechol. The calculations were carried out by GAUSSIAN 03 code.

At the first stage of electrooxidation of pyrocatechol, one electron is lost to form a corresponding π-cation radical. The unpaired electron is completely delocalized along the benzene nucleus with minor contributions on the oxygen atoms of OH groups. In a radical cation, the length of the O–H bonds is much longer and makes up to 0.997 and 1.107 Å than in a neutral molecule [3]. When the next electron is lost, a singlet π-cation is formed, the positive charge of which is strongly delocalized throughout the benzene nucleus. The O–H bond is activated before the proton is eliminated, as evidenced by a slight increase in the bond to 0.981 Å and a strong electrostatic polarization of the OH bond. However, it is assumed that the cleavage of the second proton is more energy-consuming than the first proton because the OH bond in the cation at the penultimate stage is less elongated than that of the cation radical at the initial stage of electrooxidation.

The values of the total energy of molecules and intermediates (E_{tot}), the value of the dipole moment (μ), and the frequency of the first oscillatory mod (ν_1) in the IR spectra of compounds according to the mechanism under study are given in Table 1. The orientation of the vector of the molecule's dipole moment is shown in Fig. 1.

Molecule (ion, radical)	electronic state	E_{tot}, a.u.	μ, D	ν_1, cm^{-1}
1	^1A	-382.68974	3.28	181
2	^2A	-382.50590	3.76	142
3	^2A	-382.05841	6.36	147
4	^1A	-381.85214	6.42	98
5	^1A	-381.45121	7.08	78

Table 1. The total energy, dipole moment, and frequency of the first oscillation in the IR specters of compounds are **1**-**5**.

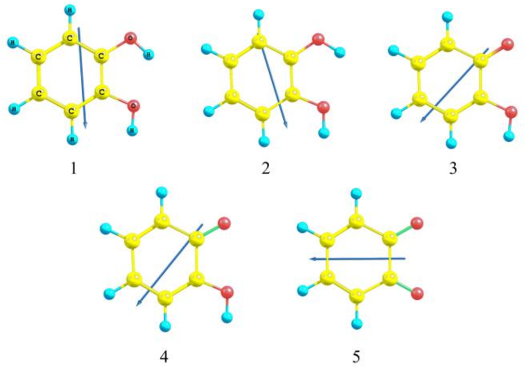

Figure 1. The direction of the dipole moment vector in a series of compounds **1**-**5**

Cation radical **2**, radical **3**, and cation **4** are π-electron in nature with significant spin localization on Oxygen atoms of the side CO and OH groups. The formation of cation radical **2** and cation **4** activates the OH bond to the proton cleavage, as evidenced by the increase in the length of this bond relative to neutral pyrocatechol **1** and radical **3** [4].

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P61

Viscosity in water from first-principles and deep-neural-network simulations

We report on an extensive study of the viscosity of liquid water at near-ambient conditions, performed within the Green-Kubo theory of linear response and equilibrium ab initio molecular dynamics (AIMD), based on density-functional theory (DFT). In order to cope with the long simulation times necessary to achieve an acceptable statistical accuracy, our ab initio approach is enhanced with deep-neural-network potentials (NNP). This approach is first validated against AIMD results, obtained by using the Perdew–Burke–Ernzerhof (PBE) exchange-correlation functional and paying careful attention to crucial, yet often overlooked, aspects of the statistical data analysis. Then, we train a second NNP to a dataset generated from the Strongly Constrained and Appropriately Normed (SCAN) functional. Once the error resulting from the imperfect prediction of the melting line is offset by referring the simulated temperature to the theoretical melting one, our SCAN predictions of the shear viscosity of water are in very good agreement with experiments. https://www.nature.com/articles/s41524-022-00830-7

P62

Vibrational spectroscopy in metallic systems

A new interest in employing Infra-Red Spectroscopy (IRS) for studying vibrational properties in metals aroused in the last decades. There exist a variety of systems where the intense electronic response that characterized the low-energy spectrum of metals does not obliterate the other excitations features in the region. A small free-carriers density or a short electronic lifetime (due for example to a strong electron-phonon cou- pling), hinter the electronic response enough for the vibrational and the structural signature of the material to become experi- mentally accessible. A strong electron-phonon interaction is the property that allow the high-Tc BCS superconductivity of hydrides under ultra-high pressure (UHP). Moreover, the UHP apparatus prevents most techniques for sample characteriza- tion except IRS, making super-hydrides the perfect candidates for this measurement. I would present the ab-initio DFT ap- proach and the computational strategy I adopted to simulate the H3 S spectrum published in Capitani et al., Nat. Phys. (2017).

P63

The semi–classical swing: classical atomic oscillations in a quantum liquid.

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Within Many–Body Perturbation theory it is well known that a quantized classical atomic oscillation (phonon) acquires an intrinsic energy indetermination (line–width). The *semi–classical swing* is, instead, a mixed classical quantistic system where the classical harmonic oscillator is not quantized and immersed in a quantistic fermionic liquid. In practice any theory based on the Born–Oppenheimer approximation can be linked to a specific approximated solution of the *semi–classical swing.*

In this poster I will discuss the *semi–classical swing* physics showing that it is an elemental out–of–equilibrium system. Its physics allows to explain several key concepts of equilibrium and out–of–equilibrium systems and, in particular, the link between relaxation and fluctuation.

I will provide a sketch of the mathematical justifications and approximations and provide numerical results and links to the existing litterature.

P64

Magnetic excitations in combination with externally applied electric field or internal crystal field effects

We report recent developments for the ab-initio study of magnetic excitations, in combination with externally applied electric field or internal crystal field effects. The adiabatic magnon spectrum is calculated starting from a Green's function / relativistic multiple scattering approach, within the framework of density functional theory. Landau damping is incorporated through a parameter-free approximation of the transverse Stoner susceptibility. The calculation scheme is applied to ferromagnetic metals as thin films over a semi-infinite substrate, and to a conducting antiferromagnetic oxide in bulk. Both the dispersion and the Stoner-limited lifetime of the magnon eigenmodes show in the two examples the effect respectively of the externally applied Efield perturbation, and of the combination between spatial and time-reversal symmetry.

P65

Solids that are also liquids: the elastic tensors of superionics from first-principles strain fluctuations

Superionics are a fascinating class of materials displaying both solid- and liquid-like characteristics: as solids, they respond elastically to shear stress; as liquids, they exhibit fast-ion diffusion, and require sampling of the configurational space to estimate expectation values. Here [1], we apply the strain fluctuations method of Parrinello and Rahman to derive the elastic tensors of benchmark superionics from first-principles molecular dynamics in the isothermal isobaric ensemble. Statistical errors are calculated through a block analysis, and zero-temperature and room-temperature tensors are extracted from simulations at different temperatures using Wachtman’s law. Finally, a comparison to static approaches sampled over a trajectory is discussed, highlighting overestimations in the range 25%-50%. [1] G. Materzanini, T. Chiarotti, and N. Marzari, "Solids that are also liquids: Elastic tensors of superionic materials", npj Comput. Mater., in press (2022).

P66

Molecular dynamics strategies to determine the melting curve of CaO

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The thermodynamic properties of multicomponent liquids at high pressure and temperature (HP-HT) are of paramount importance to shed a light on the melting and crystallization phase relations in geological systems. At the required extreme conditions of high pressure and high temperature, though, experiments suffer from uncertainties of hundreds of K and rarely predict the ultimate nature of melting [1]. Ab initio molecular dynamics (AIMD) already gave useful insights on the structure-energy properties of solid and liquid phases up to very HP-HT conditions, but the calculated melting temperature (T_m) depends critically on the simulation protocol and the computational cost increases proportionally with the number of atoms to process.

In this work we focus on the melting curve of CaO, not only because is a key phase in material and geological sciences, but also because the thermodynamic properties of the liquid phase are still controversial due to the very high melting point of the crystal [1,4]. The simplicity of its phase diagram makes it a good candidate for AIMD simulations, which are, however, very time consuming, while classical MD with empirical potentials allows to employ different strategies at a reasonably low computational cost.

We simulate the melting process of CaO with classic molecular dynamics, employing the LAMMPS code [5]. We tested three different methods, which gave insights both on the melting temperature of the crystal and on the enthalpy of fusion (ΔH_f).

The two-phase solid-liquid coexistence method consists of running a solid-liquid interface at constant enthalpy [3,6]. The melting temperature is determined as the average equilibrium temperature.

The void-nucleated method exploits holes in the crystal structure to initiate the melting process, thus decreasing the unrealistic high melting point resulting from homogeneous heating simulations by introducing a defect [2].

Finally, to calculate the enthalpy of fusion, the temperature of the crystal is increased up until the solid melts, and then the temperature is lowered again until the liquid phase recrystallizes. The difference in energy between the liquid and the solid curves at the melting point represents the enthalpy of fusion, ΔH_f [2].

The values of T_m and ΔH_f obtained with these methods by the means of classic MD on CaO are found to be consistent with experimental data available in literature [7,8].

Employing the two-phase solid-liquid coexistence method, we also calculated the high-pressure melting curve of CaO up to 30 GPa, a result which represents a starting point for the construction of a completely theoretically predicted HP-HT phase diagram of the system.

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P67

Interstitials of binary rock salt compounds

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The energetic and mechanical stability of interstitial point defects in binary rock-salt materials was studied using first-principles methods. A novel, stable, and energetically competitive interstitial site (base-interstitial) was identified for anion interstitials in rock salts. The formation energies of base-interstitial defects were compared with well-explored tetrahedral (body-interstitial) and split interstitials and were found to be highly competitive energetically. For alkali halides and silver bromide, the lowest formation energies are associated with the base-interstitial site together with the <110> split interstitial, and these are therefore the predominant interstitial sites. However, in metal monochalcogenide systems, split interstitials were found to be the energetically preferred configuration. Electronic band structures are affected by the presence of interstitial defects in rock-salt structures. In particular, the Fermi level is shifted below the valence band maxima for the body, base, and split interstitials in metal halides, indicating p-type conductivity. However, the Fermi level remains within the bandgap for metal monochalcogenides, indicating no preferred conductivity for base- and split-interstitial defects. Allowing the defects to be charged changes the relative stability of the interstitial sites. However, for alkali halides, the new base-interstitial site remains preferred over a range of potentials. The discovery of a new interstitial site affects our understanding of defects in binary rock salts, including structure and dynamics as well as associated thermodynamic and kinetic properties that are interstitial dependent.

Ab initio studies of hybrid organic–antiferromagnetic interfaces: the case of pentacene on NiO(001)

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Organically functionalized solid surfaces have acquired a fundamental role in many fields of research, thanks to the remarkable flexibility of organic chemistry in tuning the molecular electronic and optical properties. The latter can, in turn, modify the properties of the solid substrate. As an example, in "spinterfaces" – i.e. interfaces between a magnetic material and a layer of organic molecules – the molecular layer can tune the spin polarization of the substrate surface [1], with potential applications in spintronics.

In this work I will report on a first-principles study of the structural, electronic and magnetic properties of pentacene molecules adsorbed on the NiO(001) surface. The work is part of the FET-Open Project SINFONIA, devoted to the investigation of hybrid interfaces between organic molecules (ORG) and antiferromagnetic materials (AF). Calculations are performed by exploiting plane-wave DFT with Hubbard-correction, as implemented in the QuantumEspresso code. We first investigate adsorption geometries for pentacene on NiO(001), considering different possible surface supercells, molecular orientations and adsorption sites, guided by the available experimental information. Once selected the most stable configurations for molecules adsorbed on either thick or ultrathin NiO, we analyze their electronic properties, and the modifications of both molecule and surface magnetic moments upon adsorption.

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P69

Computing the phase diagram of strongly anharmonic crystals. CsSni3: the route to eco-friendly solar cells

Substituting fossil fuels with renewable sources is one of the main challenges of our society, and perovskite solar cells (PSCs) are among the most promising solutions for energy harvesting. However, the most efficient PSCs contain highly toxic lead. CsSnI$_3$ could be a promising eco-friendly alternative thanks to the excellent optoelectronic properties of its black perovskite phase, but its deployment into general markets is hampered by the rapid phase changes of samples exposed to air. Here, we simulate with first principles the finite-temperature phase diagram of CsSnI_3, highlighting how it is exceptionally driven by the quantum and thermal anharmonic motion of ions. Thanks to the state-of-the-art treatment of anharmonicity, our simulations have a remarkable agreement with experimental data both in the transition temperatures between the orthorhombic, rhombohedral, and cubic perovskite structures and the thermal expansion coefficient. Our results provide unexpected insights into the stability of CsSnI_3, establishing that the black perovskite is actually stable at room temperature and that its decomposition into the yellow phase, detrimental for photovoltaic applications, can be prevented with appropriate surface treatment and crystal growth. The simulations also disclose a singular decrease of the heat capacity upon heating of CsSnI_3 and dispel the claims on the significant role played by the rattling motion of the Cs^+ cation on the structural instability.

P70

Anharmonic Phonons From Path Integral Molecular Dynamics Simulations

Hydrogen-rich materials are characterized by large quantum fluctuations affecting hydrogen motion. While the impact of nuclear quantum effects (NQEs) on the behaviour of these systems is substantial, from the theoretical and computational sides understanding how NQEs modify their vibrational properties still represents a challenge. In this poster, I present a framework that we have recently introduced to compute accurate phonons in atomic and molecular crystals even in case of strong quantum anharmonicity. This method is based on the evaluation of the static limit of the exact phononic Matsubara Green's function. Our approach is fully ab-initio, as we obtain this quantity within density functional theory coupled with path integral molecular dynamics. We show that one can reach converged phonon frequencies at much lower computational cost and at higher precision than previously reported in literature. As application, we show the vibron modes of phase III of solid molecular hydrogen and phonon dispersions of the superconducting H3S with unprecedented accuracy.

P71

ATOMISTIC STUDY OF AN IDEAL THERMOELECTRIC CONTACT: THE FULL – HEUSLER / HALF – HEUSLER INTERFACE

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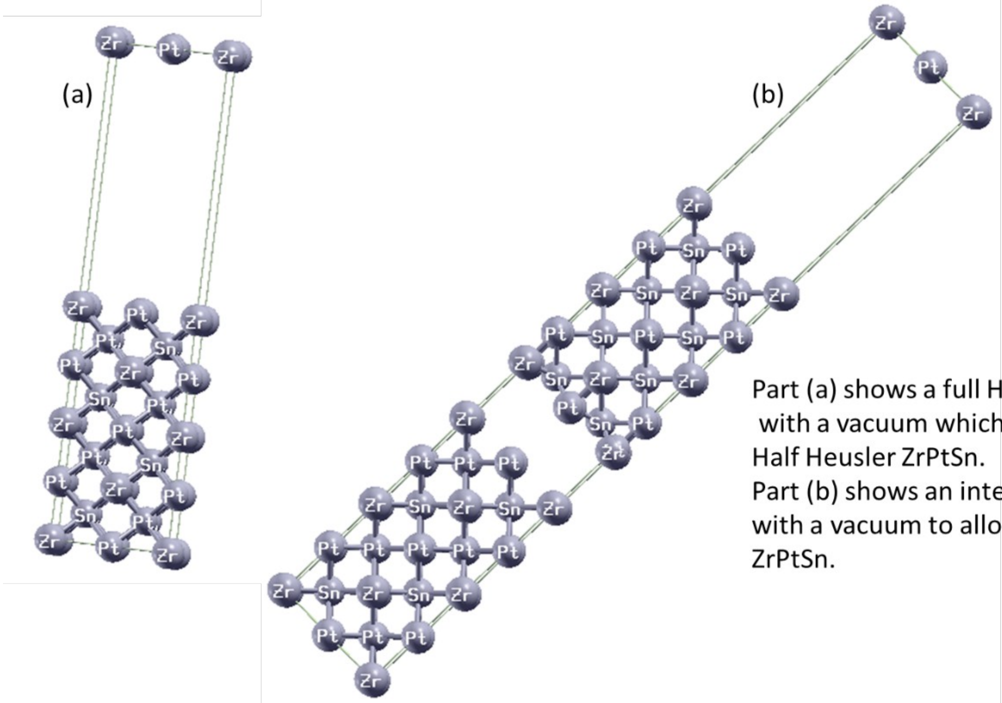
Abstract

Half Heusler alloys such as the ZrPtSn compound are important thermoelectric materials for converting waste heat into electricity. Reduced electrical resistivity at the hot interface between half Heusler material and a metal contact is critical for device performance, however, this is yet to be achieved in practice. Recent experimental work suggests that a coherent interface between half Heusler and full Heusler compound can form due to diffusion of transition metal atoms into the vacant sub lattice of the half Heusler lattice. We study computationally the structural and electronic properties of such an interface using first principle based approach that combines *ab initio* calculations with macroscopic modeling. We find that the $ZrPt_2Sn$/ZrPtSn interface provides very low contact resistivity and almost ohmic behavior over a wide range of temperatures. Given that the potential of this interface remain stable over a wide range of temperatures, our study suggests that the full Heusler $ZrPt_2Sn$ might provide nearly ideal electrical contact to the half Heusler ZrPtSn. This interface can be harnessed for efficient thermoelectric generator devices.



Part (a) shows a full Heusler ZrPt2Sn structure with a vacuum which should be occupied by the Half Heusler ZrPtSn.
Part (b) shows an interface of ZrPt2Sn/ZrPtSn with a vacuum to allow diffusion into ZrPtSn.

P72

Tuning of MoS2 band structure with atom intercalation during synthesis

P73

Effect of N & C sites vacancy defects in (G/h-BN) HS of 2D materials

Abstract

Heterostructures (HS) and vacancy defects in HS of 2D materials are fervently inspected for a profusion of applications because of their aptness to form stacked layers that confer approach to an amalgamation of favorable electronic and magnetic properties. In this study, we investigated the structural, electronic, magnetic and transport properties of N & C sites vacancy defects in G/h-BN HS material by using first-principles calculations based on spin-polarized density functional theory method within van der Waals (vdW) corrections DFT-D2 approach. We found that these considered materials are stable 2D vdW HS. Band structure calculations of these materials reveal that N site vacancy defected G/h-BN material has semimetallic nature. On the other hand, 1C vacancy defected G/h-BN material has semiconducting properties. On the basis of density of states and partial density of states calculation, the defective systems have magnetic properties. Transport properties of considered materials are examined by using BoltzTrap package and found that both materials have good thermal properties and hence they will use in thermoelectric materials.

P74

Structural prediction of group IV monochalcogenides and their pressure-induced transitions mechanism: Evolutionary algorithm and ab-initio calculations

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Sn-X and Ge-X (X = S, O) are candidates for future functional materials in semiconductor technologies. However, only the SnS phase diagram has been intensively investigated. Our knowledge of the SnO and GeS phase diagrams is still limited. There are few systematic theoretical investigations of pressure-induced transitions in SnS, GeS, and SnO, due to the difficulty of a priori the possible phases. Using a combined DFT and genetic algorithm, we systematically explored the structural diversity and phase stability under ambient conditions and high pressure. Our study identified the multiple structural transitions of SnO and PbO upon compression, including novel phases. Novel phases of SnS and GeS with attractive electronic and optical properties are predicted. The phase transitions of Sn-X and Ge-X at high pressure were found to consist of several intermediate metatransitions. Lone pair delocalization and elastic instability are the main drivers for these pressure-induced phase transitions.

P75

Selective oxidation of ethylene glycol on transition metal oxide under dry and humid conditions from ab-initio molecular dynamics approach

Nowadays, the fight for green and environmentally friendly energy is on the rise. The main reason why it is essential to switch to an organic fuel such as ethylene glycol on which catalytic oxidation results in the formation of a harmless product such as water or carbon dioxide. Using an ab-initio molecular dynamics approach, we report the oxidation of ethylene glycol on a transition metal oxide under both dry and wet conditions with particular interest in selectivity. We find that under dry conditions, the chemical reaction occurs only for a maximum coverage of 6 glycols on the B-terminated cobalt oxide (001) surface. Upon addition of water molecules in the gas phase in the presence of 4 glycols on the same B-terminated surface (001), deprotonation occurs from the glycol to the surface to form a hydroxyl group and we also noticed a proton transfer by the Grotthus mechanism. This proton transfer occurs between water molecules and from water to the surface with a localized character as a function of the increase in the number of water molecules.

P76

An ab initio supercell approach for high-harmonic generation in liquids

Many important ultrafast phenomena take place in the liquid phase. However, there is no practical theory to predict how liquids respond to intense light. Here, we propose an $ab~initio$ accurate method to study the non-perturbative interaction of intense pulses with a liquid target to investigate its high-harmonic emission. We consider the case of liquid water, but the method can be applied to any other liquid or amorphous system. The liquid water structure is reproduced using Car-Parrinello molecular dynamics simulations in a periodic supercell. Then, we employ real-time time-dependent density functional theory to evaluate the light-liquid interaction. We outline the practical numerical conditions to obtain a converged response. Also, we discuss the impact of nuclei ultrafast dynamics on the non-linear response of system. In addition, by considering two different ordered structures of ice, we show how harmonic emission responds to the loss of long-range order in liquid water.

P77

Lattice dynamics and electron-phonon coupling in $Fe_{1-x}Co_xGe$: effects of magnetism

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A study of the effect of magnetism on the lattice dynamics and the electron-phonon coupling for the solid solution $Fe_{1-x}Co_xGe$ $(0 \leq x \leq 1)$ is presented. For this, first principles calculations have been carried out, by means of the Density Functional Perturbation Theory (DFPT), using the Mixed Basis Pseudopotential method (MBPP) in two different phases: non-magnetic (NM) and ferromagnetic (FM). In particular, the evolution of the magnetic moment as a function of the Co-content (x) in the solid solution is analyzed, as well as its connection with the induced changes in the phonon frequencies. Special emphasis is placed on the phonon linewidth for specific high-symmetry directions and different frequency ranges, in order to determine the influence of magnetism on the lattice dynamics.

P78

Ab initio Molecular Dynamics Study of 2-propanol Oxidation at Co3O4(001)/H2O Interface

The catalytic properties of the Co3O4 spinel for partial oxidation reactions have stimulated a great deal of interest in recent years. In order to gain insight into structure-activity relationships, the oxidation of 2-propanol can serve as a probe reaction. This reaction is simple enough to be studied in detail, yet sufficiently complex to provide selectivity for several possible reaction products. However, many such catalytic reactions take place not in the gas phase but rather in aqueous solution, for which knowledge in the literature is relatively limited. Therefore, we performed ab initio molecular dynamics simulations in order to study the oxidation of 2-propanol at the Co3O4 (001)/H2O interface. In particular, we investigated the impact of solvation, surface termination, electrochemical environment, temperature and reactant concentration. It is shown that 2-propanol mainly adsorbs molecularly on Co3O4 (001) surfaces. However, dissociative adsorption on pristine surfaces is also observed to a minor extent. The adsorption sites for both terminations of Co3O4 (001) surface are reported. The B-termination is found to be favourable for 2-propanol oxidation as a consequence of the formation of an ordered epitaxial water layer. A hydrogen-deficient environment can also trigger the oxidation reaction. Proton exchanges are facilitated at an elevated temperature of 450 K. Near the interface, water is a double-edged sword: on the one hand, it can promote 2-propanol oxidation by providing mobile OH group in the adsorbate layer and subsequent deprotonation of 2-propanol. On the other hand, water competes with 2-propanol molecules for adsorption sites and also reduces the surface reactivity by proton transfer to lattice oxygen atoms.

P79

Theoretical Studies On Investigation Of Gas Adsorption and Sensing On 2-Dimensional Surfaces

It is well established that studying the adsorption of many gas molecules from first principles is important nowadays since it assists in predicting the feasibility of sensing (and storage) of environmentally significant gases on various surfaces. Recently, there has been an increase in the screening of various suitable materials as adsorbing surfaces in this direction. In this regard, we investigate the adsorption of gases, particularly, H2, CO, and NO, on pristine two-dimensional (2D) aluminene and transition metal (TM=Ti, Cr, Fe, and Co) atom substituted aluminene surfaces employing van der Waals dispersion corrected density functional theory. By estimating the adsorption energy (Eads) and examining the Bader charges, the energetics and the extent of charge transfer occurring between the adsorbate and surface have been discussed. The Kubas interaction has been found to have a crucial role in stabilizing H2 adsorption on TM-substituted systems. The bonding between the molecules and the TM atom through the frontier orbitals (of molecules) explains the CO and NO adsorption on TM-aluminene surfaces. Furthermore, the positioning of the TM d-band centre and the TM d-bands spread help in describing the reactivity trend for TM-aluminene surfaces for CO/NO adsorption. The evaluation of recovery time (Rt) and the change in the electrical conductivity after the gas adsorption reveal that the H2 adsorbed systems have smaller Rt values and demonstrate the greatest change in electrical conductivity. As a result, TM functionalized surfaces may serve as reusable H2 gas sensors and efficient substrates for H2 gas storage. Moreover, the surfaces may have potential for efficient disposable gas sensors when exploited for the adsorption of CO and NO gas molecules.

P80

Effects of Solvation on Reduction of Carbon Dioxide on Copper Electrocatalyst

Carbon dioxide (CO_2) is one of the major causes for global warming. Electrochemical reduction of CO_2 using renewable sources of electrical energy into valuable chemical feedstock offers an attractive solution as it solves both energy and environmental issues at the same time. In the present study, the process of electrochemical CO_2 reduction on Cu(100) surface was investigated by multiscale modelling, including DFT and kinetic Monte Carlo simulations. Results of the DFT part of the study show that one of the main products of the CO_2 reduction and the crucial intermediate in the production of hydrocarbons, carbon monoxide (CO), is formed via the carboxyl pathway ($CO_2 \rightarrow$ trans-COOH* $\rightarrow$ cis-COOH* $\rightarrow$ CO* + OH* $\rightarrow$ CO* $\rightarrow$ CO). Additionally, solvation effects of all elementary reactions involved in the process were studied and results show that both intermediates and adsorbates are more stable when solvated. Finally, data obtained in the DFT calculations was used for the kinetic Monte Carlo simulations in order to obtain detailed surface coverage, catalytic performance, and turnover frequency of the whole catalytic process.

P81

Hydrodynamic contributions to the thermal conductivity of amorphous materials in the infinite-size limit

In the past few years, the theory of thermal transport in amorphous materials has been extended beyond the Allen-Feldman formulation and unified with lattice dynamics methods for crystals within the Green-Kubo linear response theory. The computational effort required by those methods usually scales as the cube of the number of atoms, thus severely limiting the range of sizes of glass models one is able to investigate. By leveraging hydrodynamic arguments, we show how this issue can be overcome by means of a simple formula to extrapolate a reliable infinite-size estimate of thermal conductivity from glass models with a few hundred atoms.

P82

GW multipole approach for the frequency description of the dielectric screening in metals

The plasmon pole approximation (PPA) is the most common model for the frequency dependence in GW. It has been successfully applied to a large variety of systems ranging from the homogeneous electron gas, insulators and semiconductors, and simple metals. However, metals with small plasmon energies have complex frequency dependencies and often require full frequency approaches, even if computationally expensive. In this work, we explore the use of a multipole approach (MPA) in order to overcome the limitations of PPA for metallic systems. MPA has been recently developed and validated for semiconductors [1], with a particular focus on optimal sampling strategies in the complex frequency plane. In the present work, we optimise the sampling to better fit the case of metals and propose a simple method to include the intra-band contributions with small momentum transfer. The good agreement between MPA and full frequency results for the calculations of quasi-particles energies, polarizability, self-energy and spectral functions in different metallic systems confirms the accuracy and computational efficiency of the method. 1. D. A. Leon, C. Cardoso, T. Chiarotti, D. Varsano, E. Molinari, and A. Ferretti, Phys. Rev. B 104, 115157 (2021)

P83

The Evolution of Vibrational Modes of FeSe Under Uniaxial Strain

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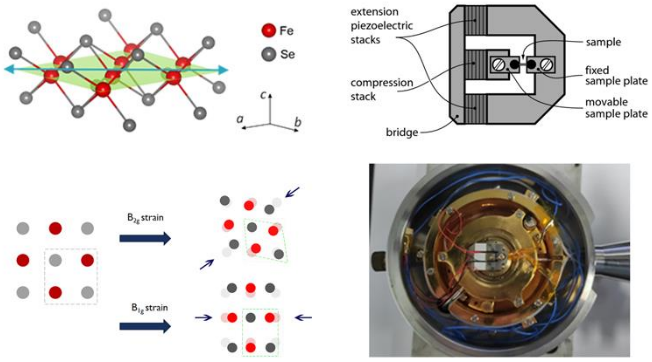
Application of strain is one of the effective ways to engineer the various properties of materials. Iron-based superconductors are suitable materials to study the strain dependence of physical properties due to their high sensitivity to variations in the local crystal structure. Among the iron-based superconductor family, FeSe is a prominent example of the interplay between superconductivity, magnetism, and electronic nematicity, which can be tuned both by chemical substitution and by application of physical pressure and consequent lattice distortions [1].

Here we present a first principle study of evolution of vibrational modes of the strained FeSe. We performed a systematic computational study, using density functional theory formalism, on bulk FeSe crystals with applying the in-plane uniaxial strain in B_{1g} and B_{2g} symmetry channels, in the range -1.5% to 1.5%. For the calculation, we used the experimental parameters and the volume cell of the unit cell is conserved under applied uniaxial strain [2].

We focus on the effect of the modification of the lattice constant, and the consequent symmetry distortion, on characteristic A_{1g} and B_{1g} modes of FeSe. These findings are compared with experimental data from Raman measurements, studying the trend of changes of A_{1g} and B_{1g} modes with applied strain using a piezoelectric strain device. The sample was mounted in such a way that the strain was applied in the *ab*-crystallographic plane and that the direction of incident light propagation is along the crystallographic *c*-axes. The sample orientations were set so that [110] (B_{2g}) and [100] (B_{1g}) crystallographic directions were orthogonal to a gap between the holder plates.

The work was supported by the Science Fund of the Republic of Serbia, PROMIS, No. 6062656, StrainedFeSC [3].



Left: Schematic representation of applied strain, Right: piezoelectric strain device, schematic and photography

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[3] http://strainedfesc.ipb.ac.rs/

Title: Elucidating the chiral anomaly in Dirac materials via electronic structure calculations

Authors: Elizabeth A. Peterson, Christopher Lane, Jian-Xin Zhu

Topological materials such as those with Dirac or Weyl dispersion are not only of fundamental interest but also have significant technological implications. In recent years, evidence for a chiral anomaly has been experimentally observed in the layered Dirac semimetal ZrTe5. Experimental transport and ARPES measurements have demonstrated that a Lifshitz transition characterized by a change from p-type to n-type carriers occurs in ZrTe5 with decreasing temperature, as evidenced by an anomalous peak in the longitudinal resistivity and a change in sign of the Hall coefficient at the transition temperature. The source of the transition is suspected to be the chiral magnetic effect, which is supported by the observation of negative longitudinal magnetoresistance. Recently attention has turned to less-well-studied, isostructural HfTe5, a 3D massive Dirac fermion system with nearly linear bulk band dispersion. HfTe5 also exhibits evidence of a Lifshitz transition and a chiral anomaly, making understanding of its electronic structure important for understanding this phenomenon in this class of materials. Here we use density functional theory calculations to identify the role of spin-orbit coupling by considering a series of isostructural MTe5 materials, and then proceed to probe the effect of strain, and Te vacancies, which are suspected to proliferate, on the electronic structure of HfTe5, on the band structure and topology, with a goal to elucidate the transport properties of this material in the presence of a magnetic field.

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P85

Orbital Hall effect in 2D Dirac materials

rbitronics has been recently emerged as very active topic research after several proposals where the aim is to exploit the orbital degree of freedom. In this communication we describe the appearance of orbital-related physics in 2d materials, in particular topological insulators and heterostructures. We start by considering the Kane-Mele model system where a topological transition is achieved by tuning some model parameters, we show that in this case the orbital moment behaves differently depending on whether the system is in the trivial or topological state. We next show the simula- tions from realistic systems where the Orbital Hall conductivity has been calculated through Kubo Formula, along with the spin Hall conductivity. The results obtained for realistic systems well dis- played overall the features obtained from the model system enabling us to claim general arguments about the appearance of orbital physics in these systems. We conclude by commenting the impact of disorder on the Orbital transport once a simple Anderson-type disorder is introduced.

P86

Ab initio modelling of alloyed superconductors from statistical thermodynamic models

Pedro Pires Ferreira, Roman Lucrezi, Christoph Heil, Luiz Tadeu Fernandes Eleno Computational Materials Science Group (ComputEEL/MatSci), Universidade de São Paulo, Escola de Engenharia de Lorena, DEMAR, Lorena, Brazil Institute of Theoretical and Computational Physics, Graz University of Technology, NAWI Graz, 8010, Graz, Austria With the present work, we propose the thermodynamic statistical modeling of alloyed superconducting systems through an extended generalized quasichemical model fully ab initio. The generalized quasichemical approximation (GQCA) considers the system as an ensemble of individual clusters statistically and energetically independent of the surrounding atomic configuration. In that way, one can evaluate any physical property of disordered systems through an average of the individual cluster properties weighted by the cluster occurrence probabilities which minimizes the overall mixing free energy. We extend that model by analytically including the vibrational free energy and applying it to metallic systems, particularly superconducting compounds. As a proof of concept, we use the extended GQCA for the well-known Al-doped MgB$_2$. Employing the conventional and perturbative density functional theory formalisms, we investigate how the structural parameters, the density of states at the Fermi level, phonon frequencies, electron-phonon coupling, and superconducting critical temperature evolve with the Al composition, showing a remarkable agreement with the available experimental data.

P87

Exploring novel chalcogen perovskite for ultra low thermal conductivity and high mobility

Chalcogen perovskite have gained attention for addressing the challenges regarding halide perovskite containing toxic element and instability in moisture. These materials holds promise for energy conversion application given its notable optical and electrical properties. Recently, chalcogen perovskite attracts the scientific community for thermoelectric due to their large seebeck coefficients and ultra-low thermal conductivity. We investigated an emerging orthorhombic chalcogen perovskite, SrZrS3, which is promising TE material by using first-principles calculations combined with the semiclassical Boltzmann transport theory with VASP and QE software. Our calculation reveals that the bang gap from HSE and GW0 are 2.05 and 2.27 eV respectively. The SrZrS3 shows excellent thermal stability , which leads to worthier performance of electric and thermal conductivities simultaneously; thus it possesses excellent power factor and ultra-low thermal conductivity yields impressive ZT values.

P88

High-throughput identification of electrides via automated AiiDA workflows

Electrides are a unique class of materials where some of the electrons occupy interstitial spaces in the crystal lattice. This leads to interesting materials properties, such as having a low workfunction - making them excellent electron emitters - or high catalytic activity. Here, we present the results obtained from applying an AiiDA automated workflow for electride identification to a database of over 25k materials drawn from the experimental databases ICSD, COD and MPDS, and relaxed at the PBEsol DFT level. We identify 352 new electrides, including a number of non-metallic candidates that can display electride behaviour under appropriate doping. The search also includes magnetic systems, for which we notably identify 33 new electrides with a difference in the density distributions of the interstitial charge of each spin channel, thus providing an exciting platform for spintronic applications.

P89

Optical Response and Hot Carrier Dynamics simulations for High Photoconversion in monolayers of Tellurene

An appropriate band gap and long relaxation times for photoexcited hot carriers are some of the features required from a good candidate for photovoltaic applications. In this talk, using of ab initio many-body perturbation theory, including the spin–orbit interaction, we investigate the photocarrier generation and dynamics in α-Tellurene [1]. We show that photoexcited electrons are mainly generated in the near-infrared range, forming excitons that are strongly bound, compared to its bulk counterpart. We also explore the role of the electron–phonon and electron-electron interactions in the relaxation of charged carriers. We find that the electronic states in the first conduction band minimum couple weakly with phonons, yielding longer hot electron lifetimes, and mean free paths up to 37 nm. We also show that the extraction of hot holes may result in a challenging task as these carriers possess sub-3 nm mean free paths. We finally estimate that 1-nm-thick α-Te provides a short-circuit current density of 6.7 mA/cm2 and a maximum power conversion efficiency of 4.4%, comparable to other layered materials, which highlights its potential for efficient photovoltaic device development. [1] C. E. P. Villegas and A. R. Rocha, J. Phys. Chem. C 2022, 126, 14, 6129–6134 (2022).

P90

Multiscale molecular modelling for applications on bioenergy energy with carbon capture and storage

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Bioenergy Energy with Carbon Capture and Storage (BECCS) is a set of strategies to couple biomass energy production with carbon capture and storage. In this context, a sub-product of ethanol production from sugarcane is a large amount of pure CO2, being essential to capture and sequestrate CO2 efficiently and is carried out over multiple scales. A more sustainable and long-term alternative for carbon capture and storage can be on geological sites, particularly clays mineral, which is commonly available near Ethanol production plants. Clays are interesting due to their low cost, naturally abundant, and can adsorb considerable amounts of CO2. Here, we explore capture and sequestration processes using multiscale molecular modelling for BECCS applications. Our approach ranges hierarchically from first-principles calculations, molecular dynamics, lattice Boltzmann and geological models. From the carbon capture perspective, we explore the role of water in the CO2 uptake in the fluorhectorite smectite clays because of their potential for CO2 storage due to their swelling capacity. The work synergetically combines experimental and simulation for a better understanding of CO2 uptake in clays [1-3]. On the sequestration side, this work aims to provide a complete multiscale molecular to build reservoir-scale models involving CO2 mineralization processes. The multiscale molecular simulations can provide key physicochemical properties of the fluid-rock interface, CO2 diffusivity, steps of mineralization reactions and phase changes of the geological components of the formation. These implemented methodologies and findings can lead to process optimization for CO2 storage in the subsurface coupling nano to macro scales with Total Energy tools.

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P91

Anomalous transport in itinerant van der Waals ferromagnets FenGeTe2 (n = 3, 4, 5)

Ferromagnetic (FM) semimetals FenGeTe2(n = 3, 4, 5), exhibit several symmetry-protected band- crossing points or lines near the Fermi energy (E F) and topology of energy bands lead to interesting transport properties. We perform a comparative study of transport and magnetic properties of these materials employing the first-principles calculations and the tight-binding Hamiltonian is con- structed by fitting the energy bands obtained from the first principles calculations. In the presence of spin-orbit coupling (SOC) and finite magnetic moment in all three materials break the time re- versal symmetry, and for n = 3,5 system large Berry curvature (BC) is concentrated on the nodal lines. The consequence of the correlation of topological nodal line and finite magnetic moments on anomalous Hall conductivity (AHC) σxy and anomalous Nernst conductivity (ANC) αxy have been investigated. We note that σxy for n = 3, 4, and 5 at 0 K are 150, 295, and 90 S/cm, respec- tively, while the calculated ANC property αxy for n = 3, 4, and 5 are 0.55, 0.80, and 0.10 A/Km at room temperature. Our calculated AHC values at 0 K are 150 S/cm , 295 S/cm and 90 S/cm for Fe3GeTe2 ,Fe3GeTe2 and Fe5GeTe2 respectively, whereas, experimentally observed values reported values for Fe3GeTe2 is 150 S/cm i.e This is consistent with experimental values. The experimen- tally reported value of ANC for Fe3GeTe2 is close to our calculated value of 0.55 A/Km at room temperature. The calculated values of magnetic moments of all three systems are consistent with experimentally reported values.

P92

Self-consistent anharmonic phonon dynamics

Vibrational spectra, optical response, non-linear effects and pump-probe spectroscopies depend on the dynamical nuclear response to external perturbations. The Time-Dependent Self-Consistent Harmonic Approximation (TDSCHA) describes the static and dynamical properties of molecules and crystals in the Born-Oppenheimer regime accounting for quantum, anharmonic and thermal fluctuations in a non perturbative way. We reformulate TDSCHA in the Wigner framework. This clarifies the physical meaning of the equations of motion. We find that, just by changing the initial condition, TDSCHA switches between classical and quantum description of ionic motion. In addition we extend the method's capabilities, shading light on all possible scattering processes. Linearization of the equations of motion allows to compute Infrared and Raman spectra, including full anharmonic interactions between phonons and non trivial couplings with the electromagnetic field, such as two-phonon effect firstly discussed by Rasetti and Fermi. As a numerical test we present the IR spectra of high pressure hydrogen at T = 0 K and P = 250 GPa where these effects are relevant.

P93

Strain control of the competition between metallic and semiconducting states in single-layers of $TaSe_3$

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Since the discovery of graphene in 2004, there has been a huge improvement in the fabrication and manipulation of layered materials. Importantly, the discovery that a monolayer of MoS_2 changes its electronic properties with respect to the bulk brought much expectation in the scientific community towards transition metal chalcogenides (TMCs). MX_2 transition metal dichalcogenides (TMDCs) have been thoroughly studied both experimentally and theoretically in the past years. Nowadays, TMCs with different chemical stoichiometries such as the transition metal trichalcogenides (TMTCs) MX_3 are also being intensely studied. Interestingly, semiconducting TMTCs such as TiS_3 have already been investigated [1,2] and it has been found that it is possible to tune its electronic and optical properties by means of strain.

In this work [3], we have shifted our attention towards a metallic TMTC, $TaSe_3$. This material has been subject to several studies in the past due to its appealing properties that could be used in future applications. Although the monolayer structure of $TaSe_3$ is expected to have a semiconducting behavior, we found that it is not the case. In fact, it presents an interesting competition between metallic and semiconducting states under the effect of strain. By applying different types of strains we found that the metallic state can be modified depending on whether the application of the strain is biaxial or uniaxial either along the short or long range directions of the layer. Importantly, we saw that it is possible to stabilize a semiconducting state when applying a uniaxial strain along the long direction of the layer. Furthermore, this gap can be tuned by changing the strength of this tensile strain. Therefore, we have shown that $TaSe_3$ is a very versatile system that could be used in novel devices. Moreover, the fact that its bulk counterpart exhibits superconductivity makes future studies of this material even more appealing.

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P94

Engineering the trend of the thermal conductivity of solids

The temperature dependence of the thermal conductivity of crystals and glasses generally exhibits opposite asymptotic trends, decreasing as 1/T in the former and increasing (often up to a saturation value) in the latter. These originate from different microscopic conduction mechanisms: particle-like propagation of atomic vibrational waves in crystals, and wave-like tunneling between vibrational modes in glasses. Recently, it has been shown that these two mechanisms naturally emerge from a unified Wigner formulation of transport, raising fundamental questions on their coexistence and on related potential applications. Here, we show that the relative strength of particle-like and wave-like conduction mechanisms can be regulated by varying the degree of structural disorder or the strength of anharmonicity, practically allowing to engineer the magnitude and trend of the temperature-conductivity curve. We demonstrate these findings by quantum-accurate calculations of thermal transport in solids with variable degree of disorder and anharmonicity, providing evidence that temperature-conductivity curves with trends intermediate between the 1/T decay of crystals and the increasing trend of glasses can be obtained. References: Simoncelli, M., Marzari, N. & Mauri, F. Unified theory of thermal transport in crystals and glasses. Nat. Phys. 15, 809–813 (2019). Simoncelli, M., Marzari, N. & Mauri, F. Wigner formulation of thermal transport in solids. Accepted in Phys. Rev. X, preprint at http://arxiv.org/abs/2112.06897 (2022). Simoncelli, M., Mauri, F. & Marzari, N. Thermal conductivity of glasses above the plateau: first-principles theory and applications. preprint at http://arxiv.org/abs/2209.11201 (2022).

P95

The activation of p-orbital for nitrogen fixation

Electrochemical reactions have to utilize catalyst materials to achieve high performance, and numerous catalyst materials are essential for various types of reactions. The activity of present catalysts is generally thought to be related with the d-orbital of the transition metals, while the electronic modulation of p-orbital of the metal elements was rarely reported. Here we propose a general approach to modulate the 6p-orbital of Bi element to design the catalyst for nitrogen fixation reactions. the existence of Bi2+ and Bi2+ in the Bi system rather than the pure Bi or Bi3+ could effectively inject electrons from the half-occupied pz of Bi2+ into N2. The unique p-orbital electronic structure of Bi plays a vital role in it. This work sheds light for the modulation of p-orbital of main group elements.

P96

Theoretical characterization of the trap states in quasi-stoichiometric amorphous $Ge_xSe_{(1-x)}$-based chalcogenides with different chemical doping

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ABSTRACT

Amorphous chalcogenide materials have been attracting an increase attention as typological candidates for the resistor and select elements in non-volatile three-dimensional (3D) stackable phase-change memories with a crossbar array architecture; such as for instance recently integrated in 3D X-point memory by Intel. A particular interest has been devoted to amorphous GeSe based-chalcogenide due mainly to its suppleness of undergoing both non-volatile resistance and Ovonic threshold switching (OTS)[1]. However, the implementation of amorphous GeSe in such device structures is still suffering from low thermal stability at high temperature and drop in its electrical response. To overcome such issues, the variation in the chemical stoichiometric of amorphous $Ge_xSe_{(1-x)}$ or the incorporation of chemical dopants demonstrated a significant improvement in its thermal stability and electrical properties, which yield a higher GeSe-based ovonic threshold switching selector performance[2]. However, the mechanism behind such improvement is still not understood and unclear. Here, we perform a systematic study by using a material-to-device multiscale technique to efficiency characterize the active trap states within the gap mobility of amorphous $Ge_xSe_{(1-x)}$. Such technique combines together the classical molecular dynamics (MD) simulations, density functional theory calculations, experimental measurements and device characterizations of the key features of $Ge_xSe_{(1-x)}$ amorphous. Furthermore, we vary the chemical stoichiometric in the amorphous $Ge_xSe_{(1-x)}$ as well as we incorporate Si, Te, S and P atoms as chemical dopants to encompass different existing experimental scenarios. Our combined approach can be useful for development and optimization of any other amorphous-chalcogenide-based device technologies.

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P97

Unconventional linear flexoelectricity in two-dimensional materials

We present a general first-principles formalism to calculate the macroscopic polarization response of a two-dimensional (2D) material to a flexural deformation. The characteristic flexoelectric coefficients are expressed as linear-response quantities within the framework of the long-wave DFPT [1,2,3,4] and can be calculated with the primitive cell of the flat configuration. Interestingly, we find that the 2D geometry allows for tensor components that are forbidden at the bulk level: inversion-symmetric hexagonal crystals (e.g., monolayer SnS2, bilayer BN, silicene, phosphorene, SnS2 and RhI3) yield a nonvanishing in-plane polarization response to bending. This means that, by folding a 2D material of these characteristics into a zigzag nanotube, a net current travels along the axial direction that is proportional to the curvature; conversely, in an armchair nanotube, the current circulates along the perimeter. Our first-principles calculations show that the corresponding flexoelectric response is much larger than the out-of-plane one, [4] in several cases almost an order of magnitude larger. We validate our linear-response method by performing direct calculations of the axial Berry-phase polarization of a SnS2 nanotube, finding excellent agreement. [1] Miquel Royo and Massimiliano Stengel, “First-principles theory of spatial dispersion: Dynamical quadrupoles and flexoelectricity,” Phys. Rev. X 9, 021050 (2019). [2] Massimiliano Stengel, “Flexoelectricity from density-functional perturbation theory”, Phys. Rev. B 88, 174106 (2013). [3] Miquel Royo and Massimiliano Stengel, “Exact Long-Range Dielectric Screening and Interatomic Force Constants in Quasi-Two-Dimensional Crystals” Phys. Rev. X 11, 041027 (2021). [4] Matteo Springolo, Miquel Royo, and Massimiliano Stengel, “Direct and Converse Flexoelectricity in Two-Dimensional Materials” Phys. Rev. Lett. 127, 216801 (2021).

Artificial-Intelligence-Guided Workflow for the Accelerated Discovery of Metal Oxide Water Splitting Catalysts Using Beyond-DFT Calculations

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Developing strategies to discover potential catalysts which can facilitate water splitting reaction is a need of the hour to deal with the current energy crisis.[1] In spite of the large number of materials scrutinized, the expected water splitting efficiency has not been achieved so far. Transition metal oxides (TMOs) have employed as efficient catalysts for water splitting.[2] However, the large number of TMOs reported so far and the inadequacy of traditional DFT methods to accurately treat the catalytically important properties are two important challenges in materials space exploration of water splitting catalysts. Recently, data-driven approaches such as machine learning (ML) and Artificial Intelligence (AI), have emerged as important tools for conducting large scale catalysts discovery.[3] Nevertheless, the conventionally practiced black-box ML models often confront challenges in the acquisition of high-quality data and their predictions suffer from interpretability issues.[4] In this regard, we have conducted a materials space exploration of TMO based water splitting catalysts using beyond-DFT calculations and Artificial Intelligence (AI) methods. By applying a beyond-DFT approach based on accuracy upgraded hybrid functionals, methodological improvement for accurate stability as well as electronic structure prediction of TMOs is achieved. Based on a multi-fidelity model based active learning AI approach, an automated workflow is developed for accelerated material discovery. The sure independence screening and sparsifying operator (SISSO) based AI model revealed the crux features of TMOs in governing their stability and activity under catalytically relevant conditions.[5] The obtained atomistic level understanding of material properties and the developed workflow could be extended for other problems of renewable energy interest.

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Understanding the structure of amorphous chalcogenides for improving their electrical performances

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Amorphous chalcogenides, such as GST and GeSe, are emerging materials employed in the design of innovative non-volatile electronic memories. They can change their phase (Phase Change Materials, PCM), from amorphous to crystalline, or conduction state (Ovonic Threshold Switching, OTS) depending on the current that flows through them.

The structural and electrical properties of these chalcogenides are strongly related to the presence of short- and medium-range structures in the amorphous phase that are responsible for the internal structural orders at different length-scales. In order to deeply understand the local geometry-dependent properties of these chalcogenide systems, we employed a combined approach based on both classical molecular dynamics (MD) simulations and ab-initio calculations.

To obtain the structural features of chalcogenide systems in the amorphous phase, MD simulations containing thousands of atoms have been employed and simulated for hundreds of nanoseconds. The simulated structures were analyzed using cutting edge techniques and theories based on the chemical/physical and topological approaches shedding light on how the different percentages of atomic types affect the order at different lengths[1].

In order to compute the electronic properties of amorphous systems, we developed a procedure to extract several configurations of few hundreds of atoms from the extended structures obtained from MD simulations. The results show that a small difference in the stoichiometry affects not only the mobility band-gap size, but also the number and the position of the trap states with respect of the mobility edges.

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P100

High-throughput computational screening of fast Li-ion conductors

We present a high-throughput computational screening to find fast Li-ion conductors to identify promising candidate materials for application in solid-state electrolytes. Starting with ~30,000 experimental structures sourced from COD, ICSD and MPDS repositories, we performed highly automated calculations using AiiDA at the level of Density Functional Theory (DFT) to identify electronic insulators and to estimate lithium ion diffusivity using the pinball model which describes the potential energy landscape of diffusing lithium at near DFT level accuracy while being orders of magnitude faster. We present the workflow where the accuracy of the pinball model is improved self-consistently and which is necessary in automatically running the thousands of required calculations and analysing their results. Promising conductors are further studied with first-principles molecular dynamics simulations.

P101

X-ray spectrocopy theoretical spectra of Gold in Warm Dense Matter regime

The prediction and analysis of optical and X-Ray spectra of materials allows to obtain information about the electronic structure and electronic transport properties, especially in "Warm Dense Matter" regime in which direct observables are hardly accessible. In this perspective, the Kubo-Greenwood formula associated with the PAW approach has proven its efficiency to compute these properties on large disordered systems possibly with vacuum (expansion). We recently added the spin-orbit coupling contribution in the formalism [1] and are now able to compute the XANES (X-ray Absorption Near Edge Spectroscopy) L edges of transition metals independently and coherently, in a fully ab initio scheme. We present theoretical computations of XANES spectra near L edges for Gold. We show that XANES experiments associated with DFT calculations are a powerful tool to investigate metals (possibly in two-temperature conditions) and to link their ionic and electronic properties.

P102

Hidden Magnetoelectric Multipoles, and anti-Magnetoelectric Effect in α-Fe_2O_3

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We present first-principles calculations of hidden order, in the form of hidden magnetoelectric multipoles, in Cr_2O_3 and its iron-based analogue, α-Fe_2O_3. We show that in the prototypical magnetoelectric material Cr_2O_3, the linear magnetoelectric effect, in which an applied magnetic field induces a linear electric polarization, or an electric field induces a linear magnetization, can be interpreted in terms of the ferroic ordering of magnetoelectric multipoles. In centrosymmetric α-Fe_2O_3, which has the same crystal structure as Cr_2O_3 but a different magnetic ordering, our calculations reveal hidden anti-ferroically ordered magnetoelectric multipoles. We predict an anti-magnetoelectric effect in α-Fe_2O_3, in which pairs of spins cant in opposite directions under the application of an external electric field, to create an additional anti-ferromagnetic ordering. We confirm the predicted spin canting using first-principles methods, showing that the study of hidden magnetoelectric multipoles can be used to reveal previously unknown effects.

P103

A computational study on the opto-electronic properties of various AuRh nanoclusters obtained through different synthetic processes

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The growing interest in gold-based nanoalloys arises from the possibility of combining the optical features of gold with the catalytic capabilities of other transition metals, leading to a new generation of highly-effective photocatalysts.[1] Among the many alloys, AuRh nanosystems are extremely promising since they can successfully catalyse several essential reactions: hydrogen generation from water,[2] oxygen evolution,[3] and hydrogenation of double bonds.[4] Nothwithstanding its relevance, not many studies focused on AuRh. Our work aims to clarify the relation between ionic structure, chemical ordering and opto-electronic features of AuRh nanoalloys which size ranges from 20 to 150 atoms. We employ a multiscale numerical approach, combining classical Molecular Dynamics (MD) with Density Functional Theory (DFT) and Time-Dependent Density Functional Theory (TDDFT) calculations. We compare three formation processes in the gas-phase: the one-by-one growth, the coalescence between two nanoclusters, and the annealing of nanoalloy droplets. As a general trend, we recover a significant predominance of Rh@Au core-shell ordering over random and Janus-like. This tendency is confirmed by the reordering of random and Janus-like configurations into core-shell geometries on a timescale shorter than one ns at 600-800K. At classical level, we identified some "magical sizes" corresponding to specific geometrical closure with enhanced thermal stability and used them as starting configurations for our DFT and TDDFT studies. A Rh_{19} seed can adopt a double-icosahedron or an icosahedron-decahedron shape dynamically. A novel $Au_{52}Rh_{19}$ geometry, with Au forming a chiral monolayer around a double-icosahedron Rh_{19}, is a very stable isomer with a melting temperature of about 1000K. Globally, this work unravels some unique and notable features of AuRh nanoalloys and represent a guide for further studies in this field.[5]

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P104

Lithium adsorption on the interface of graphene/boron nitride nanoribbons

It has been shown that combining 2D materials in vertical or lateral heterostructures can significantly change and improve their electronic properties, making them more applicable for various purposes, e.g. nanoelectronics, spintronics, energy storage, catalysis etc. In this work, first principle calculations have been employed to investigate the influence of Li adsorption on lateral heterostructures composed of nanoribbons of graphene (gr) and hexagonal boron nitride (hBN). The results indicate the profound role of the nanoribbon interface, where the severe changes in in the electronic band structure occur. Indeed, hybridisation of electronic states induces bangap opening of about 0.2 eV in the boron terminated zigzag gr-hBN nanoribbon, thus showing that tuning electronic properties can be acomplished by Li adsorption.

P105

Boron carbide under torsional stress at 5 GPa combined to density functional theory (DFT) calculations: evidence of the formation of chain vacancies in the plastic regime driven with the rotating tomography Paris Edinburgh cell (RoToPEC)

The behaviour of boron carbide under stress/deformation has been a long-standing puzzle with, on the one hand, outstanding static mechanical properties, and on the other one, a shear strength in the shocked state that rapidly decreases beyond the Hugoniot elastic limit, resulting in premature failure of the material as the shock stress reaches a threshold value of 20 GPa. Several explanations have been put forward: phase transition, occurrence of shear bands containing amorphous solid, formation of chain vacancies followed by carbon-carbon bond reformation at high pressure. In the present work, damage and point defects generated with the RoToPEC have been identified at ambient pressure by energy dispersive X-ray microdiffraction, Raman spectroscopy, and DFT calculations of atomic structures and phonon frequencies. We show that apart from the signals due to B_4C, new peaks appear in both characterisation methods, and that most of them can be attributed to boron atom vacancies in the intericosahedral chains of boron carbide, as predicted in Ref. [1]. Some of the Raman spectra also show peaks that have been attributed to amorphous boron carbide in the literature. Deformed boron carbide thus shows small inclusions of clusters of B_4C, with chain vacancies, and/or small zones interpreted as amorphous zones [2]. [1] R. Raucoules, N. Vast, E. Betranhandy, J. Sjakste, Physical Review B 84, 014112 (2011). [2] A. Chakraborti, A. Jay, O. Hardouin Duparc, J. Sjakste, K. Béneut, N. Vast, Y. Le Godec, Acta Materialia 226, 117553 (2022). Results have been obtained with the Quantum ESPRESSO package. Computer time has been granted by PRACE Project No. 2019204962 and by French GENCI-CINES and GENCI-TGCC (Project 2210), Support from DGA and NEEDS-Matériaux is gratefully acknowledged.The PSICHE beamline in SOLEIL synchrotron and the Raman spectroscopy platform in IMPMC are also acknowledged.

P106

Topology-induced giant piezoelectricity in conjugated polymers

Thanks to the possibility they offer to convert mechanical energy into electrical energy and vice-versa, piezoelectric materials are of great interest in various fields and find many applications, ranging from macro- to microscopic electromechanical devices, to energy harvesting and much more. For their high electromechanical response, the most widely used piezoelectric materials are inorganic perovskites, such as lead zirconate titanate (PZT). However, they present some limitations since they have very low mechanical flexibility, high fabrication costs and are often toxic because of the lead they contain. A promising alternative is to exploit piezoelectric properties of organic materials. In our work, we focus on conjugated polymers, a peculiar class of organic materials, and propose a mechanism that allows to enhance their piezoelectric response exploiting their topological properties. Our predictions are supported by density functional theory calculations and suggest a possible direction in order to outperform the inorganic counterparts.

P107

Genetic-tunneling driven variance controlled energy optimizer for monolayer magnetic materials at finite temperatures

Novel topological spin textures, such as magnetic skyrmion benefit from its inherent stability, acting as the ground state in several magnetic systems. Currently, in the study of atomic monolayer magnetic materials, reasonable initial guesses are still needed for searching those magnetic patterns. This situation underlines the need to develop a more effective way to identify those non-trivial textures. To solve this problem, here we propose a genetic-tunneling driven variance-controlled optimization approach, which combines local energy minimizer back-end and metaheuristic global searching front-end. This algorithm is an effective optimization solution for searching magnetic ground states at low temperatures and is also robust for searching low-energy degenerated states at finite temperatures. In this sense, we show the success of this method in searching magnetic ground states with both artificial and real 2D monolayer systems without prior knowledge. It is also worth noting that the inherent concurrent property of this algorithm can significantly speed up the study of topologically protected textures in magnetic materials. In conclusion, the method we proposed here builds a new type of paradigm for low-dimensional magnetic system energy optimization.

P108

Plasmon dispersion in 3D type-I Dirac material Li3Bi

Electron-hole excitations in a material can give rise to a collective charge excitation, called plasmon, which is the key property for many applications in the field of plasmonics. Dirac plasmons in novel topological semimetals, which are the three-dimensional counterpart of graphene have attracted great interest [1]. Li3Bi is layered material with band structures that host Dirac point and shows type-I dispersions near the Fermi level, offering an ideal platform to investigate Dirac plasmons. So far, the predictions of Dirac plasmon properties, such as the existence of novel long- lived gapless plasmons, have been based mostly on simplified models representing the band dispersion only around the Dirac points [2]. In this work, instead, on the basis of ab initio time-dependent density-functional theory simulations, we take into account both the contributions from the whole band structure and the effects of the electron-hole interaction. We obtain an accurate and realistic description of the plasmon dispersion in this compound, which allows us to draw a detailed picture of plasmon properties in different types of Dirac topological semimetals. This work is done in collaboration with Ridwan Agbaoye (Nigeria), Maram Ali Ahmed (Sudan), Timothy Ashani (Nigeria), Bruno Dandogbessi (Nigeria), Wala Elsayed (Rowanda), Mohamed Kinawy (Egypt), Menberu Woldemariam (Ethiopia), Andrea Marini (Italy), Matteo Gatti (France).

P109

Rotational g factors and Lorentz forces of molecules and solids from density-functional perturbation theory

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Applied magnetic fields can couple to atomic displacements via generalized Lorentz forces, which are commonly expressed as gyromagnetic g factors. We develop an efficient first-principles methodology based on density-functional perturbation theory to calculate this effect in both molecules and solids to linear order in the applied field. Our methodology is based on two linear-response quantities: the macroscopic polarization response to an atomic displacement (i.e., Born effective charge tensor), and the antisymmetric part of its first real-space moment, denoted as $\mathbf{J}^{(\mathbf{1})}$ in this work (the symmetric part corresponding to the dynamical quadrupole tensor). The latter quantity is calculated via an analytical expansion of the current induced by a long-wavelength phonon perturbation, and compared to numerical derivatives of finite-wavevector calculations. We validate our methodology in finite systems by computing the gyromagnetic g factor of several simple molecules, demonstrating excellent agreement with experiment and previous density-functional theory and quantum chemistry calculations. In addition, we demonstrate the utility of our method in extended systems by computing the energy splitting of the low-frequency transverse-optical phonon mode of cubic $\mathrm{SrTiO_3}$ in the presence of a magnetic field. The formalism presented in this work opens exciting avenues for magnetic field effects in lattice dynamics of both finite and extended systems. First, the molecular g factors obtained with our DFPT-based methodology compare well with the best theoretical values from the literature, obtained via much more expensive computational approaches. And second, our results demonstrate that the contributions to phonon g factors in solids coming from $\mathbf{J}^{(1)}$, which had been neglected in earlier studies, dominate the response in the case of cubic $\mathrm{SrTiO_3}$.

P110

Effect of uniaxial strain on the excitonic properties of monolayer C_3N

In recent years, the application of mechanical stress has become a widespread experimental method to tune the electronic and optical properties of two-dimensional (2D) materials. In this work, we investigate the impact of uniaxial tensile strain along zig-zag and armchair directions on the excitonic properties of graphene-like C$_3$N, a single layer indirect-gap material with relevant mechanical and optical properties. Both dark and bright excitons have been computed for different strain configurations, by solving a model Bethe Salpeter Equation (BSE), based on a tight binding (TB) description of the valence and conduction bands involved in the lowest lying excitons. We use this model approach to classify excitons of pristine and strained C$_3$N according to the crystal symmetry and to explain the appearance of bright excitons with intense optical anisotropy in strained C$_3$N, even at small strains. Finally, the effect of strain on the exciton dispersion at small centre of mass momenta will be also discussed.

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Anharmonicity and lattice dynamics in the structural phase transition of perovskite oxides

It is challenging to study crystalline materials such as perovskite ceramics that have a structural phase transition with increasing temperature. In this study, we predicted the phase transition temperature Tc of some oxides using machine learning interatomic potentials and temperature-dependent anharmonic lattice dynamics simulation. Our predictions for Tc are comparable with experimental values. We found that these materials are highly anharmonic and the frequency of the phonons strongly depends on the temperature. Finally, using temperature-dependent interatomic force constants and molecular dynamics simulations, we calculated their lattice thermal conductivity, which is very different from the calculation using zero-temperature interatomic force constants.