Vienna Ab-initio Simulation Package (VASP) Ecosystem

Book of Abstracts

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Opening Talk

Best practices using VASP: Parallelisation and HPC resources

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In this talk I will discuss the parallelisation strategy VASP employs to distribute its work and data, and the ways a user may influence these to optimise the performance of VASP on high-performance computing (HPC) resources, be it CPU-only or GPU-accelerated hardware. The main focus will be on aspects of the parallelisation using MPI, but I will briefly touch upon the use of MPI + OpenMP as well.

Day 1 - Session 1

Predicting and understanding phase stability using lattice-dynamics modelling (IT)

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The stability of a material is an important consideration, particularly in systems with multiple competing phases, and is an area where modelling can provide valuable input to experiments.

However, a typical athermal DFT calculation on an equilibrium structure only yields the lattice energy, which provides limited scope for investigating stability. The theory of lattice dynamics, which accounts for the natural thermal motion (phonons) in periodic systems, provides an efficient means to address this issue by incorporating temperature effects into calculations.

Phonon frequency calculations within the harmonic approximation (HA) can be used to compute the phonon contribution to the temperature-dependent Helmholtz free energy, which can be used to compare the relative stability of materials as a function of temperature. The quasi-harmonic approximation (QHA) further takes into account the effect of volume changes to compute the Gibbs free energy, which is in most cases a more experimentally-relevant quantity, and can also predict the effect of applied pressure.

Finally, lattice-dynamics calculations also provide a means to assess dynamical stability based on the presence or absence of imaginary harmonic frequencies in the phonon spectrum. In some cases, imaginary modes may identify an unstable structure or a failed geometry optimisation, whereas in others they can provide insight into the structural relationship between phases and the mechanism of the transition between them.

In this talk, we will illustrate the applications of these models to a number of topical systems, including the tin chalcogenides Sn_xS_y/Sn_xSe_y and the archetypal hybrid halide perovskite $(CH_3NH_3)PbI_3$.

Influence of alloying elements on phase stability in nickelbase superalloys (CT)

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Several intermetallic phases are important in the design of Nickelbase superalloys: The γ'-phase (Ni3Al) and γ''-phase (Ni3Nb) provide strengthening whereas the δ-phase (Ni3Nb) and η-phase (Ni3Ti) are important in ensuring a fine-grained structure in wrought alloys, but may also be detrimental because they may embrittle the alloy.

The solution energies of all transition elements in all possible positions of the four phases are calculated. It is shown that it is possible to model these energies using two quantities, the Bader charge and the atomic volume in a nickel matrix. We also show how a high concentration of Cr or Co in the matrix stabilizes these phases by increasing the energy of the phase-forming element in the matrix. Finally, we discuss the influence of magnetic effects and provide some insights in how to overcome convergence problems.

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Anharmonic lattice dynamics and phonon transport in extended solids (CT)

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Computation of lattice dynamics including anharmonic effects at a given temperature is critically important for describing phonon transport in extended solids, accurately. I will showcase with few examples, how temperature dependent effective potential (TDEP) method [1] in combination with ab-initio molecular dynamics (AIMD) simulations aid to describe the anharmonic lattice dynamics, consequently, accurate description of phonon transport in low lattice thermal conductivity (kl) materials. Designing materials with an ultralow kl is of paramount importance for thermal energy management applications. For instance, several strategies have been proposed to achieve ultralow kl, among them, the interplay of lone pair, layered structure, mass contrast between constituent elements in a material provide a pathway for engineering anharmonicity, bonding heterogeneity, flat and soft phonon bands to increase phonon-phonon scattering channels to suppress kl [2-4]. Layered materials consisting of a lone pair cation with mass contrast [4,5] aid to design ultralow kl materials. However, AIMD simulations are computationally very demanding, therefore, we adopt methodology training on-the-fly machine learning force fields (MLFFs) using AIMD simulations [6]. The MLFFs allow us to perform MD simulations for longer time and length scales within classical MD simulation time close to ab-initio accuracy. This would enable us to predict the properties of materials at finite temperatures, which remains as a longstanding problem in computational materials science.

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Day 1 - Session 2

Ultrafast control of complex oxide functional properties: New insights from theory and electronic structure calculations (IT)

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Recent experiments have demonstrated the potential for ultrafast changes in the functional properties of materials upon selective optical excitation of particular phonon modes. The chemical diversity of complex oxides, and their strong lattice-properties coupling, have made them ideal test systems for new experimental approaches that exploit anharmonic phonon couplings to induce and modify magnetism, superconductivity and ferroelectricity with light. In this talk, I will describe our recent theoretical efforts exploring ultrafast optical control of the functional properties of perovskite oxides. First, I will describe the theoretical framework that we have developed, and the role of electronic structure calculations in that framework. I will then focus on an example of our framework in action: dynamical stabilization of a non-equilibrium magnetic phase in GdTiO3. Finally, I will consider how to identify materials that may exhibit a large dynamical response and present our results of a systematic exploration of intrinsic materials factors that may contribute to the nonlinear phononics response in LaAlO3. Our work highlights the importance of understanding the contributions of small structural distortions to the optical response in perovskites (in contrast with large-amplitude distortions, such as octahedral rotations), and illustrates how anharmonic mode coupling strengths may not be the most important factor in which materials exhibit large or unusual responses, as has generally been assumed.

Lowering lattice thermal conductivity in Barium chalcogenides through lattice expansion (CT)

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Understanding thermal transport is of fundamental importance in several technological applications, like transistors, optoelectronics, photovoltaics, and thermoelectrics. Materials with an intrinsic low lattice thermal conductivity (kl) provides a pathway for discovering high zT materials without degrading its charge transport. Lattice expansion is one of the strategies to achieve low kl through phonon softening. In the present study, the effect of lattice expansion on the phonon transport properties of Barium Chalcogenides has been studied. Dynamical stability of these compounds under lattice expansion has been established from the computed phonon dispersion curves. A significant lowering of lattice thermal conductivity (5.63 Wm-1K-1 to 2.06 Wm-1K-1, 6.17 Wm-1K-1 to 2.38 Wm-1K-1, 9.84 Wm-1K-1 to 5.1 Wm-1K-1) for BaO, BaS and BaTe respectively with increasing lattice expansion from 0% to 4% was observed. Microscopic origins for low lattice kl are discussed through phonon scattering and phonon group velocities. Current research could provide insights into how to develop low kl materials by lattice expansion, which is crucial for developing sustainable energy conversion systems for future thermal energy applications.

Lattice Dynamics in Ferrimagnetic Layered van der Waals Material $Mn_3Si_2Te_6$ (CT)

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$Mn_3Si_2Te_6$ single crystals were first synthesized in 1985 1, however, few studies were carried out on this compound since. It was only recently that the attention has shifted to them, mainly through the comparisons with quasi-two-dimensional materials, specifically $CrSiTe_3$. Layered magnetic van der Waals materials have lately received widespread attention due to their relevnce for spintronics, magneto-electronics and data storage.
$Mn_3Si_2Te_6$ crystalizes in a trigonal $P\bar{3}1c$ crystal structure (No. 163 space group) [2]. First principle calculations suggested a competition between ferrimagnetic ground state and three additional magnetic configurations, originating from antiferromagnetic exchange for the three nearest Mn-Mn pairs [2]. Here we present a first principle study with the focus on the phonon properties [3]. We compare our computational results with experimental Raman scattering of $Mn_3Si_2Te_6$ single crystals. Eighteen Raman-active modes are identified, fourteen of which are assigned according to the trigonal symmetry. Five A_{1g} modes and nine E_g modes are observed and assigned according to the $P\bar{3}1c$ symmetry group. Four additional peaks to the ones ascribed to the $P\bar{3}1c$ symmetry group and obeying the A_{1g} selection rules, are attributed to overtones. A pronounced asymmetry of the A^5_{1g} phonon mode is evidenced at 100K and 300 K. The unconventional temperature evolution of the A^5_{1g} Raman mode reveals three successive, possibly magnetic, phase transitions that are expected to have significant impact on the strength of the spin-phonon interaction in $Mn_3Si_2Te_6$. These are suggested to be caused by the competition between the various magnetic states, which are close in energy.
This study provides a comprehensive insight into the lattice properties of the considered system and shows arguments for the emergence of competing short-range magnetic phases in $Mn_3Si_2Te_6$.
The calculations are based on the density functional theory formalism as implemented in the Vienna Ab-initio Simulation Package (VASP) [4-7], with the plane wave basis truncated at a kinetic energy of 520 eV, using the Perdew-Burke-Ernzehof (PBE) exchange-correlation functional [8] and the projector augmented wave (PAW) method [9,10]. The Monkhorst and Pack scheme of the k point sampling is employed to integrate over the first Brillouin zone with 12×12×10 at the Γ-centered grid. The convergence criteria for energy and force have been set to 10^{-6} eV and 0.001 eVÅ^{-1}, respectively. The DFT-D2 method of Grimme is employed for van der Waals corrections [11]. The vibrational modes are calculated applying the density functional perturbation theory implemented in VASP and Phonopy [12].

Application of MXenes in heterogeneous catalysis: A computational perspective (CT)

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The catalytic activities of several different heterogeneous catalysts, ranging from planar extended surfaces to clusters and particles with different shapes, sizes or compositions, have been experimentally determined for a long time. However, a fully understanding of the catalytic mechanisms is a defiant task because of the large number of variables that determine the performance of the catalyst. Therefore, to isolate the effect of each variable, studies using well-controlled conditions that allow separating the influence of different parameters in the global catalytic processes are required. Computer modelling arises as a very adequate strategy since the composition of the systems can be fully controlled, with relevant information being retrieved when combined with electronic structure methods. In this communication, we will present results

from density functional theory calculations, performed with the VASP code [1] and using the periodic slab approach, about the potential of two-dimensional carbide or nitride MXenes for heterogeneous catalysis of industrial and societal relevant processes, such as the water gas shift reaction, ammonia production or carbon capture and usage [2].

Acknowledgments
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Modelling the evolution of oxide nanoparticles in the presence adsorbed molecules (IT)

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We will consider the case of cerium dioxide, an important material in water gas shift reactions, three-way catalysis, soot oxidation, and enzyme mimetic activity (nanozymes). In such catalytic applications, the performance of the catalyst is dependent on the morphology of the nanoparticle. Control of size and morphology of nanoparticles is therefore key for the design of energy and catalytic materials as it significantly affects the surface composition, reactivity and selectivity. As different surfaces show different catalytic activity, the nanoparticles should be shaped to express those surfaces with enhanced activity. Although synthesis can achieve selective control, a key challenge is to identify strategies to enhance the expression of catalytically active surfaces and to prevent their disappearance over many catalytic cycles. Here, we use density functional theory to predict the surface composition and energetics of cerium dioxide {111}, {110} and {100} surfaces in the presence of water, carbon dioxide and hydrogen peroxide. We found that there is a strong chemical adsorption of all species. Whereas water and hydrogen peroxide display dissociative adsorption, carbon dioxide forms surface carbonates. The strength of the adsorption is surface dependent, and generally it follows the order {100} > {110} > {111}. Using a thermodynamic strategy, we then calculate the surface free energy of adsorbed surfaces as a function of external conditions. This allows us to predict changes in the equilibrium nanoparticle morphology following changes from octahedral, truncated octahedral and cuboidal shapes as a function of temperature, water and oxygen partial pressure.

Day 2 - Session 1

Light and elevated temperature degradation of silicon solar cells: How is HPC cracking it? (IT)

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Photovoltaic (PV) installations have recently reached the terawatt level and this is almost entirely due to the success of silicon-based solar cell technologies. Silicon PV is low-cost and cell efficiencies are unrivalled by other mass-market single-junction technologies. Improvements in silicon cells will have a real-world impact on climate change mitigation and improving energy supply security.

Hydrogen-related defect engineering is fundamental for several processes in the photovoltaics industry. It is involved in the fabrication of anti-reflection coatings and in the passivation of surface and bulk carrier traps. However, hydrogen has also been blamed for being involved in the degradation of the conversion efficiency of Si solar cells (by up to 16% relative after several months/years of sun-light exposure in the field). This is known as Light and elevated Temperature Induced Degradation (LeTID) of the cells, and it is manifested as a severe life-time reduction of photo-generated electrons which are trapped and annihilated at unknown defects in the silicon.

We present a hybrid density functional study of thermally- and carrier-activated processes involving reactions between hydrogen and group-III acceptors in crystalline silicon. Finite-temperature calculations of the free energy change along the reactions, allow us to come up with a first-principles-level account of the degradation mechanism of the cells, as well as possible routes for avoiding LeTID.

Our findings have important repercussions regarding our understanding of hydrogen in p-type silicon, its role on doping and lifetime of carriers.

Activation of metal-free porous basal plane of Biphenylene through defects engineering for Hydrogen evolution reaction (CT)

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The biggest challenge in the commercial application of electrochemical reduction of water through the hydrogen evolution reaction (HER) is hampered due to the scarcity of inexpensive and efficient catalysts. Herein, we propose a metal-free biphenylene nanosheet, a recently proposed two- dimensional (2D) carbon allotrope [Science 372.6544 (2021)], as an excellent HER electrocatalyst. The dynamical and thermal stability of biphenylene nanosheet is validated through phonon dispersion and ab-initio molecular dynamics (AIMD) calculations, respectively. The first-principles calculations show that the biphenylene nanosheet is a metal, having Pz orbitals at the Fermi level. At a low H coverage (1/54), the biphenylene nanosheet shows excellent catalytic activity with the adsorption Gibbs free energy (ΔG H*) of 0.082 eV. The B-doping and C-vacancy in biphenylene further improve the ΔG H* to ⊠0.016 eV and 0.005 eV, respectively. The strength of interactions between the H atom and the nanosheet is explained through the relative position of the p-band center. Our study opens new possibilities to use non-metallic porous materials as highly efficient electrocatalysts for HER.

Theoretical investigation of adatom doping of transition metal in hGY for electrocatalytic Oxygen evolution reaction (CT)

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In order to meet society's needs for drastically enhanced procedures for clean renewable energy, there is an urgent need for reliable and efficient sources. One of the most potent sources of energy for the future is electrocatalytic water splitting, which produces H2 and O2 for use in fuel cells containing hydrogen to create electricity. As a result, a lot of studies are being done on electrocatalytic water splitting, which involves two chemical reactions happening simultaneously: The Hydrogen Evolution Reaction (HER) and indeed the Oxygen Evolution Reaction (OER). The ability of the catalyst employed to conduct water oxidation, also known as the OER process, which is a step in the development of hydrogen synthesis from electrochemical water splitting, is what mostly constrains this progress (OER). Here, we use the first-principles DFT approach as implemented in the Quantum Espresso package to analyze the OER of 2D hGY monolayers with and without embedded transition metals (TM). It is crucial to perform theoretical simulations to understand the relationships between a material's electronic structure and its catalytic activity, which are now being used to forecast and create better catalysts. We believe this to be the first theoretical study describing the OER potential of the hGY monolayer. The 2D hGY has just recently been studied for catechol sensors and hydrogen storage applications. Benzene rings and carbon atoms that have undergone sp hybridization form the C-C networks that make up the 2D structure of hGY. The 2D system's huge surface area and uniform distribution of holes make it particularly stable and distinctive for a wide range of applications. Doping TMDCs using transition metals like (Au, Co, Cr, Pt, Sc) can enhance their performance for OER applications and increase their favorable prospects as compared to pure hGY. O, OH, and OOH were symbolically adsorbed on several transition metals in order to understand the exact OER mechanism. A transition metal's optimum electron transport to hGY is what causes the catalytic activity. As a consequence of the abatement in Gibb's free energy and the local work function caused by this electron transfer, H* interaction as well as adsorption are facilitated at each of the four steps in the traditional OER mechanism, enhancing the performance of the OER. Last but not least, the potential for active sites in hGY via a suitable/pertinent choice of metal dopants brings up new possibilities for specifically optimizing the catalytic activity of this material.

Multiscale modelling of piezoelectric composite materials for microfluidic pumps in implantable medical device (CT)

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The purpose of the present Density Functional Theory (DFT) study is an investigation the role of mixing level on the dielectric/ electronic properties by doping the PbTiO3 (PTO) to obtain lead Zirconium Titanate (PZT). The starting composite was prepared for the PZT ceramic which is used in numerous applications including actuators. Here, we focus on understanding the effect of Ti substitution by Zr in a 2x2x2 PTO supercell on the structural, electronic and polarization behaviour. The PTO supercell was relaxed at different Zr:Ti ratios, followed by the determination of density of states (DOS) and Bader charges for each composition. Furthermore, the effect of Zr on ions O (2p) and Ti (3d) hybridization was studied along their band gap. Our calculations for PTO found that the band gap value is around 1.69 eV while after doping with Zr it increased to 1.88eV. The spontaneous polarization was performed using the Berry phase to understand the effect on the polarization

Day 2 - Poster Session

Designing and investigation of alkali decorated graphene and boron nitride nanostructures for hydrogen storage: A first principles study

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Utilizing the density functional theory (DFT), a detailed investigation of hydrogen adsorption on pristine and alkali metal-decorated boron nitride and carbon nanostructures was conducted. Although the average adsorption energy is below the US-DOE threshold, the hydrogen adsorption on pure boron nitride system is still promising in terms of theoretical storage capacity. In the case of bilayer boron nitride, the overall hydrogen storage qualities are tunesd under the influence of an external electric field. An alkali (Li, Na) decorated (4-6-8 ring) boron nitride monolayer can have a theoretical storage capacity(TSC) of 4.9-5.5%, respectively with an average adsorption energy in the desired range. Similarly, GNR decorated with Li, Na and K possesses TSC of 3.8, 4.3 and 4.8 wt% respectively. Graphene and boron nitride vertical heterostructure also have a TSC of 5.83 wt% with an average adsorption energy of -0.22 eV/H2. In all the cases the hydrogen molecules adsorption mechanism is dominated by the feeble charge transfer and weak van der Waals interaction as observed from the charge transfer and electron density analysis.

Mechanical and thermodynamic properties of the some B2 rare-earth intermetallic compounds: Ab initio study and data mining approach

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The full-potential linearized augmented plane wave (FP-LAPW) method has been employed within the generalized gradient approximation (GGA) to investigate the structural and thermo-elastic properties of some rare earth intermetallics such as YAg, YCu, HoCu, LaAg, LaZn, ErCu, ErAg, ErAu, DyCu, NdAg, LaCd, YIn, and LaMg compounds. The calculated ground state properties such as lattice constants, bulk modulus and elastic constants agree well with the experiment. For HoCu and LaZn compounds, the thermodynamic properties are predicted [1, 2] via the quasi-harmonic Debye model, using to predict the low-temperature behavior of the crystal. For the first time, the numerical estimation of the thermal properties is performed for these compounds and still awaits experimental confirmations. In addition, the chemical bonding of these compounds has been investigated in the light of topological analysis approach based on the theory of atoms in molecules (AIM). The relationship between several thermo-physical and mechanical properties were discussed, and analyzed with data mining techniques. The obtained results confirm that this B2-type of rare-earth intermetallic compounds have very interesting mechanical and thermal properties for structural applications.

Day 2 - Session 2

Identification and assessment of electrides (IT)

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Electrides are rare ionic compounds in which an electron does not occupy an atomic orbital but ex-ists as a free electron in a cavity of the crystal lattice. This electron behaves differently to those occu-pying

the valence state of standard materials, making electrides desirable as electron emitters,[1] non-linear optical switches,[2] superconductors,[3] battery anodes,[4] and catalysts for applications ranging from organic synthesis to CO2 splitting.[5] An electride catalyst has even been shown to significantly improve the efficiency of the century-old Haber-Bosch process recently.[6]
We use high-throughput screening and density functional theory calculations to identify undis-covered electrides among all known materials.[7] Our method recovers the compounds Ba3CrN3 and Sr3CrN3 as electrides. These ternary nitrides are the first known case of electrides containing a transi-tion metal element, which is surprising as one would expect a redox active element to accept the anion-ic electron rather than allowing its existence in the lattice. We confirm these results with single crystal experiment, validating our method and approach. [8] Besides these compounds we find more than 60 previously unknown electrides along with 4 already known, significantly expanding this class of indus-try-relevant materials.

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The Joint Automated Repository for Various Integrated Simulations (JARVIS) for novel materials discovery and design (CT)

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The Joint Automated Repository for Various Integrated Simulations (JARVIS) hosted by the National Institute of Standards and Technology (NIST) is an integrated infrastructure to accelerate materials discovery and design, motivated by the Materials Genome Initiative (MGI). JARVIS uses density functional theory (DFT), beyond DFT methods (GW, DMFT, Quantum Monte Carlo), classical force-fields (FF), quantum computation, and machine learning (ML) techniques, all publicly hosted at: https://jarvis.nist.gov. This talk will primarily focus on JARVIS-DFT, which consists of over 70,000 materials and over 1 million calculated properties, all of which are continuously expanding. Apart from other DFT databases, JARVIS-DFT contains data calculated with more robust density functionals such as meta-GGAs and van der Waals (vdW) functionals, using strict k-point and energy cutoff convergence criteria. In addition, novel properties such as solar spectroscopic limited maximum efficiency, topological properties, magnetic anisotropy and Curie temperature for 2D magnets, and superconducting transition temperatures have recently been added to JARVIS-DFT. Calculated properties in the JARVIS-DFT database have also been used as a screening criteria for more sophisticated, higher-order Quantum Monte Carlo and electron-phonon coupling calculations. This talk will also include an interactive overview of the user friendly tools of JARVIS-DFT, with the intention that workshop participants will be able to use these tools for their future research.

Non-Abelian braiding of phonons from first principles (CT)

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Non-Abelian braiding of quasiparticles can encode quantum information immune from environmental noise with the potential to realize topological quantum computation. Here we propose that phonons, a bosonic excitation of lattice vibrations, can carry non-Abelian charges in their band structures that can be braided using external stimuli. Taking some earthly abundant materials such as silicates [1] and aluminium oxide [2] as representative examples, we demonstrate that an external electric field or electrostatic doping can give rise to phonon band inversions that induce the redistribution of non-Abelian charges, leading to non-Abelian braiding of phonons. We show that phonons can be a primary platform to study non-Abelian braiding in the reciprocal space, and we expand the toolset to study such braiding processes.

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Properties of materials under high-pressure (IT)

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Properties of materials usually requires to be tuned not only for industrial purpose but also to access to a clear understanding of their origin. Here we will discuss the benefit of using the VASP code in estimating the impact of high-pressure on the magnetic and multiferroic properties of cuprates.