Research applications using Vienna Ab initio Simulation Package (VASP)

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Opening Talk

Back to the future with VASP: Core features, old and new (OT)

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The Vienna Ab Initio Simulation Package (VASP) is one of the most widely used tools for studying and predicting the properties of materials. By performing quantum mechanical simulations based on density functional theory (DFT) and many-body perturbation theory (MBPT), VASP is used to study properties such as the electronic structure, total energy, and optical spectra. Together with the incorporation of machine-learned force fields and electron-phonon interactions, VASP offers a wider range of tools with which accurate calculations can be performed. In the latest release, VASP 6.6, the range of powerful tools was expanded further, with the addition of X-ray absorption spectra from the Bethe-Salpeter equation, the constrained random-phase approximation (cRPA) for computing effective interactions in correlated materials, electron-phonon coupling with meta-GGA functionals, and support for the GRACE family of machine-learned force fields. With the addition of GPU support on Intel and AMD GPUs, alongside the existing NVIDIA support, DFT and hybrid-functional calculations can now be accelerated on a wider range of hardware. This presentation will explore some of the core features of VASP, both old and new, their application in simulating properties of different materials, as well as VASP's role in advancing research in fields such as material design, catalysis, and nanotechnology.

Session 1

Modelling point-defect equilibria and defect association in the $CuInSe_2$ chalcopyrite: native and extrinsic defects (IT)

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The $CuInSe_2$ (CIS) chalcopyrite is used commonly as an absorber material in solar-cell devices. This has prompted extensive studies of its native point defects by both experimental and computational approaches. Further work showed that this material can be self doped by its native defects depending upon the growth non-stoichiometry conditions and the exact magnitude of the elemental chemical potentials. First-principles calculations showed that copper vacancies are the main acceptor defects and the In-to-Cu antisites the most prominent donor defects [1,2]. The present study reports hybrid-functional calculations of the formation energies of the native point defects in CIS for representative regions of the CIS phase diagram. The resulting equilibrium concentrations of both ionic and electronic defects reveal the p- or n-type character of the material and the more dominant defects for various growth conditions. Defect association was also examined considering extrinsic defects such as hydrogen which is frequently introduced in solar-cell devices either by implantation or from the chemical deposition of the window layer. Trapping of hydrogen to the copper-vacancy acceptors was found to be favourable at low temperatures confirming muon-spin spectroscopy data [3]. This vacancy-hydrogen interaction leads to passivation of the electrical activity of the copper vacancies and the decrease of the p-type character of the material.

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Engineering ultra-low lattice thermal conductivity via mass contrast and bonding heterogenity: A lattice dynamics approach for advanced thermoelectrics (CT)

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Achieving intrinsically ultra-low lattice thermal conductivity (κ_L) is the cornerstone for decoupling electron and phonon transport, a necessity for advancing high-efficiency thermoelectric energy conversion and advanced thermal management technologies. This research presents a systematic first-principles investigation integrated with the Boltzmann transport equation (BTE) and coherent two-channel transport models to map the microscopic mechanisms of phonon transport across diverse structural topologies. We examine layered PbClF type systems, rocksalt IIA–VIA alkaline-earth chalcogenides, alkali halides, and bismuth halooxides to establish fundamental structure-property relationships driven by atomic mass contrast, lattice instabilities, and bonding heterogeneities. In layered PbClF-type compounds, compounds with a large axial ratio ($c/a > 2$) - such as CaBrF, CaIF, and SrIF - exhibit ultralow out-of-plane κ_l values (< 1 W/m-K). This behavior is driven by weak van der Waals (vdW) bonding and heavy Br/I atoms acting as structural rattlers . Furthermore, anomalous, counter-intuitive κ_L trends are uncovered in rocksalt IIA–VIA and alkali halide systems, demonstrating that atomic mass contrast heavily modulates acoustic-optical phonon gaps. When combined with the inherent lone-pair activity and mixed ionic-covalent bonding heterogeneity native to bismuth halooxides and ternary halofluorides, these dynamics yield a pathway for engineering earth-abundant materials tailored for solar thermal systems, electric vehicles, and future thermal energy management applications.

Magnetic Weyl semimetals in quaternary Heusler alloys: From topology to anomalous transport (CT)

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The anomalous electronic transport arising from the interplay between magnetism and band topology in topological semimetals (TSMs) has attracted considerable attention in the materials science community due to their promising applications in quantum computing, low-dissipation electronics, spintronics, and energy-harvesting systems [1]. TSMs are characterised by nondegenerate band-touching points, known as Weyl nodes, which is a hallmark feature of these systems, is the existence of symmetry-protected surface Fermi arcs that link Weyl nodes of opposite chirality within the surface Brillouin zone [2]. This work focuses on a systematic first-principles study of the electronic, magnetic, topological, and anomalous transport properties of CoRhMnSi and CoRhMnGe, quaternary Heusler compounds. Spin-polarised electronic bandstructure calculations ensure the ferromagnetic ground state and half-metallic nature in both compounds. The topological characteristics are explored using a tight-binding approach based on Wannier functions that incorporates spin-orbit coupling, revealing multiple Weyl nodes with opposite chiralities. The observation of robust, symmetry-protected surface Fermi arcs provides compelling evidence for Weyl semi-metallic behaviour in these materials. In addition, along the [001] crystallographic direction, the obtained values of anomalous Hall conductivities were -706.34 and -1300.29 S cm^{-1} for CoRhMnSi and CoRhMnGe, respectively, at 0 K. Correspondingly, significant anomalous Nernst conductivities of -4.55 and -4.75 A $m^{-1}K^{-1}$ were predicted at room temperature, exceeding those reported for several other Co-based magnetic Heusler alloys [3]. These anomalous transport outcomes with topological characteristics highlight the potential of these compounds for spintronic and thermoelectric applications.

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Anisotropic origin of ultralow lattice thermal conductivity in KCdP half-Heusler alloy at high temperature (P)

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Thermoelectric (TE) materials are known to convert waste heat into electrical energy, but their efficiency is limited by a relatively low figure of merit, zT. The present investigations examine the quasi-two-dimensional layered half-Heusler alloy KCdP to explore its potential as a thermoelectric material, using the Boltzmann transport theory. Structural and mechanical calculations show that KCdP is a brittle material, characterized by a combination of ionic and covalent bonding. Electronic band calculations show that this material exhibits anisotropic charge-carrier transport, characterized by multi-valley band extrema, resulting in a high Seebeck coefficient and electrical conductivity. The lattice thermal conductivity is calculated by accounting for three-phonon scattering and wavelike tunneling, yielding a very low value of 0.89 W/mK at 900 K, which is attributed to its high anharmonicity, as indicated by its relatively large Grüneisen parameters. Carrier relaxation-time calculations indicate that p-type doping improves charge-carrier transport. The calculated results show that this material exhibits a high figure of merit exceeding unity within an intermediate temperature range, making it a potential, environmentally friendly thermoelectric energy-conversion material. The results also show a high degree of anisotropy, with maximum efficiencies of 20.24% (2.38%) and 6.34% (2.27%) for p-type and n-type doping along the x- and z-directions, respectively, highlighting the importance of crystallographic orientation for optimizing this material for energy conversion devices.

Understanding PtRu catalyst deactivation in direct isopropanol fuel cells (P)

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Direct isopropanol fuel cells (DIFCs) have attracted increasing attention over the recent years. Namely, zero-emission electricity production, high power densities, low-toxicity and compatibility with existing infrastructures renders them advantageous over hydrogen and other organic based fuel cells. In DIFCs isopropanol is oxidized to acetone at the anode, while oxygen gets reduced at the cathode. The most efficient known electrocatalysts for isopropanol oxidation are platinum-based owing to their high selectivity for acetone formation and low overpotentials. Among them, PtRu nanoparticles have demonstrated superior performance with the highest power densities obtained so far [1]. However, at higher overpotentials, their performance rapidly declines and becomes operationally unstable. This behavior has often been attributed to acetone adsorption and the consequent blockage of active sites. However, the precise mechanism of PtRu deactivation and the origin of the initial high activity remain unclear. Here, we perform an atomistically resolved computational study to clarify these open questions.

Given that a similar deactivation has also been observed on pure platinum, we first modelled the isopropanol oxidation reaction on the simpler Pt(111) surface, which is known to be responsible for the activity of Pt [2]. To capture electrochemical effects in the oxidative potential region, grand-canonical density functional theory (GC-DFT) was employed [3]. All computations were performed using a continuum solvation model (VASPsol++) to account for the aqueous environment. In addition to the primary reaction pathway, alternative dehydrogenation routes and water oxidation were also examined. Our preliminary results indicate that acetone and isopropanol have very similar adsorption free energies. However, side-products, formed via the dehydrogenation of the methyl groups, bind significantly more strongly to the surface than acetone, which may contribute to catalyst deactivation. Building on the gained understanding of the deactivation of pure Pt and the inactivity of pure Ru (likely linked to surface oxidation) the mechanisms on PtRu alloy will be investigated.

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Session 2

From over-reactive to inactive: Oxygen coverage as the governing control parameter in MXene catalysis (IT)

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The reactivity of Mo_2C-based MXenes is strongly conditioned by the nature and extent of their surface terminations, with oxygen playing a particularly decisive role. In this presentation, we show that varying the amount of surface oxygen fundamentally reorganizes the catalytic landscape of Mo_2C, shifting the material from overly reactive behavior to an optimal catalytic window to complete deactivation.

Our analysis combines density functional theory and microkinetic calculations to examine both directions of the water–gas shift (WGS) reaction across a series of Mo_2C surfaces with controlled termination patterns. Bare Mo_2C interacts too strongly with adsorbed intermediates, producing deep adsorption wells and hindering product release. Conversely, when the surface is fully saturated with oxygen, as in Mo_2CO_2, the material becomes essentially non-reactive: Mo sites are obstructed, adsorbate binding is weakened, and dissociation steps face prohibitive barriers. Catalytic turnover emerges only at intermediate oxygen coverages, either in the presence of fluorine terminations or vacancies.

This framework clarifies why real Mo_2CT_x catalysts—characterized experimentally by mixed terminations and vacancy defects—exhibit measurable WGS activity despite theoretical predictions of inactivity for fully O-terminated surfaces. It also establishes a generalizable concept, viz. oxygen coverage acts as a tunable design parameter that governs MXene catalytic behavior rather than a passive structural feature.

By detailing how termination chemistry reshapes reaction energetics, our studies provide actionable guidance for engineering MXenes with tailored reactivity profiles and highlights the value of computational approaches in decoding termination-dependent catalytic mechanisms.

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First-principles investigation of structural, electronic, and optical properties of Brannerite-type $CeTi_2O_6$: The role of oxygen vacancies (CT)

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Cerium-based oxides are widely investigated for photoelectric and energy conversion applications due to the reversible Ce^{3+}/Ce^{4+} redox couple. However, the role of Ce 4f states in determining the electronic, magnetic, and optical properties remains insufficiently understood. In this study, we investigate the structural, electronic, and optical properties of $CeTi_2O_6$, a brannerite-type oxide, using first-principles calculations based on Density Functional Theory (DFT).

We first optimize the ideal structure of $CeTi_2O_6$ and confirm its energetic stability, before establishing that this material is an indirect-gap semiconductor. We then introduce various types of point defects in order to identify the most energetically favorable configurations and evaluate their influence on the electronic and optical properties. Our analyses reveal that the magnetism of the oxide is predominantly governed by the Ce 4f orbitals through Ce^{3+}/Ce^{4+} redox processes, and that the optical properties exhibit significant anisotropy.

Finally, a thermodynamic stability diagram is constructed to determine the chemical potential range defining the stability of $CeTi_2O_6$ with respect to competing phases. These findings provide insight into the defect-mediated tuning of its properties, highlighting its potential for applications in catalysis, optoelectronics, and energy conversion.

Interfacial charge transfer, magnetism, and topological properties in $3d/5d$ $LaBO_3/SrIrO_3$ superlattices (B = Mn, Fe, Co, Ni) (CT)

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We present a first-principles density functional theory study of *n*-type and *p*-type $LaBO_3/SrIrO_3$ superlattices (B = Mn, Fe, Co, Ni) performed using VASP. By moving across the $3d$ transition metal series, we track systematic changes in the electronic, magnetic, and topological properties of these interfaces [1, 2].

A clear trend emerges in the interfacial charge transfer. In *p*-type superlattices, charge always moves into the $SrIrO_3$ block. The strength of this transfer depends on B-Ir covalency. In contrast, *n*-type systems show two distinct behaviors based on the nominal d-occupancy of the B-site ion relative to Ir^{4+}. For B = Co and Ni, where the d-occupancy is higher than Ir^{4+}, charge flows into the $LaBO_3$ layer. For B = Mn and Fe, where the d-occupancy is lower or equal, charge transfers into the $SrIrO_3$ block instead. Consequently, the $SrIrO_3$ layer becomes nonmagnetic in *n*-type $LaMnO_3/SrIrO_3$ and $LaFeO_3/SrIrO_3$.

In the magnetic $SrIrO_3$ blocks, ferromagnetic Ir-Ir exchange and strong spin-orbit coupling generate $C = 2$ double Weyl points in the band structure. This produces a large intrinsic anomalous Hall conductivity in both *n*-type and *p*-type $LaCoO_3/SrIrO_3$ and $LaNiO_3/SrIrO_3$. For the Mn and Fe systems, we find a finite anomalous Hall effect only in the *p*-type interfaces. However, this effect is strongly suppressed in *p*-type $LaFeO_3/SrIrO_3$. There, proximity to the antiferromagnetic $LaFeO_3$ layer weakens the ferromagnetic Ir-Ir exchange.

These calculations explain recent experimental results on $3d/5d$ oxide interfaces and offer a practical guide for future measurements.

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Impact of explicit 4f electron treatment on DFT+U local magnetic fields in the rare-earth orthoferrites (CT)

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Rare-earth orthoferrites ($RFeO_3$) exhibit intricate magnetic and structural phases resulting from the complex cross-coupling between the localized (4f) and transition-metal (3d) sublattices. Modeling these systems using Density Functional Theory (DFT) presents a significant challenge due to the strong correlation and self-interaction errors inherent to localized (4f) electrons. Taking ($NdFeO_3$) as a prototypical model system, this work systematically evaluates how different pseudopotential treatments of the (4f) shell within the VASP package impact the prediction of local magnetic environments across its spin-reorientation transition (SRT).

First-principles calculations were performed using VASP within the projector-augmented wave (PAW) method and the PBE+U framework. To capture the evolution of the internal fields, we benchmarked two distinct VASP methodologies: (i) treating the Sm/Nd (4f) electrons as frozen core states, and (ii) treating them explicitly as valence states with an optimized Hubbard (U) correction combined with spin-orbit coupling (SOC) and non-collinear magnetic restraints. Positively charged hydrogen (H^+) interstitial configurations were optimized in 80-atom supercells to model muon stopping sites. Finite-size electrostatic corrections (EFNV) were applied to handle the charged defect states. The resulting local magnetic fields were extracted via MuESR software and validated against experimental zero-field muon spin rotation (muSR) and resonance ultrasound spectroscopy (RUS) data.

Our VASP calculations demonstrate that freezing the (4f) electrons in the core successfully reproduces the structural phase transitions and structural distortions observed during the SRT. However, this core approximation fails to accurately predict the magnitude and drastic orientation shifts of the local magnetic fields at low temperatures. Conversely, explicit valence treatment of the Nd ($4f^3$) configuration provides a quantitative match with the experimental (muSR) precession frequencies (57 MHz) to (101 MHz) in the low-temperature ($Gamma_2$) phase. This methodology explicitly accounts for the critical polarization contribution of the rare-earth sublattice under the exchange field of the Fe moments. Furthermore, the relaxed non-basal coordinates of the interstitial sites show a significant local lattice relaxation (0.99 angs.) (O-H) bond lengths) that directly rules out unrelaxed electrostatic approximations historically used in rare-earth oxides.

This work establishes a VASP workflow for interpreting local magnetic probes in strongly correlated Rare-earth orthoferrites. By demonstrating the absolute necessity of explicit (4f) valence optimization for tracking internal fields, this benchmark provides a theoretical framework for high-throughput screening and data-driven discovery of functional rare-earth materials.

DFT calculations of the properties of ZrN cubic nanostructures containing Mo, Ru and Pd impurities (CT)

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Uranium mononitride (UN) has been proposed as a novel nuclear fuel for next generation nuclear reactors due to its superior properties with the potential to increase the cycle length when compared to conventional nuclear fuel [1,2]. The qualification process of UN as a novel nuclear fuel is expensive and difficult mainly because of the complications of handling highly radioactive materials. For this reason, zirconium mononitride (ZrN) is used as a surrogate because of its similar crystallographic structure and thermophysical properties, while being non-radioactive [3]. As part of the nuclear fuel cycle process, uranium derived nanostructures and a wide variety of uranium fission products are naturally produced. The properties of the nuclear fuel material might drastically change due to the size and morphology of the nanostructures, and the accumulation of the fission products [4,5]. Therefore, it is important to understand the properties of ZrN nanostructures with the addition of uranium fission products to ensure its proper application as a surrogate for UN.

In this work the properties of cubic ZrN nanostructures with the addition of uranium fission products (Mo, Ru, and Pd) were studied using a computational first-principle approach based on Density Functional Theory as implemented in VASP. ZrN cubic nanostructures of three different sizes (8, 64 and 216 atoms) were considered at increasing concentration of fission products capable of reproducing the values reported experimentally for UN at high burnup. The relative stability of the cubic ZrN nanostructures was analyzed by calculating their formation energies. This indicated that structures with Mo were the most stable, showing higher stability than the pure ZrN, where the stability increased at higher Mo concentration. The structures with Ru and Pd showed less stability than pure ZrN, where the stability decreased at higher concentrations. Nonetheless, the formation energy of all structures with fission products were relatively far from zero, indicating that ZrN cubic nanostructures are capable of retain Mo, Ru and Pd with relative stability, even at considerably higher concentrations than those reported in the experiments. Calculation of the electronic properties showed that most of the structures remained conductive, like pure bulk ZrN. However, the smaller 8 atoms structures with Mo and Pd displayed semiconductor characteristics. Future calculations of ZrN cubic nanostructures with the addition of other uranium fission products like Ce and Nd will be considered using the VASP implementation of DFT+U to describe the highly correlated f-electrons.

Automated workflows for materials discovery (IT)

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Automated ab initio calculations have emerged as a powerful tool for computational materials science. These workflows offer many benefits over traditional manual approaches, including the ability to create large datasets for machine learning; however, complex materials properties such as electronic and thermal transport have proven difficult to automate. Here, I introduce our latest work developing automation tools that are easy to use and enable interoperability between density functional theory packages. I also introduce workflows for calculating electronic and thermal transport and their role in materials discovery.