2026 School on Electron-Phonon Physics and Many-body Perturbation Theory | (SMR 4221)

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P01 - ADHIKARI Surajit

Harnessing Linear and Nonlinear Optical Responses in Ferroelectric LaMoN3 for enhanced Photovoltaic Efficiency

P02 - AHAMMED Raihan

Berry Curvature-Induced Nonlinear Transport and Optical Phenomena in Quantum Materials

P03 - ALKORTA Lopetegi Manex

Symmetry-broken ground state and phonon mediated superconductivity in CsV3Sb5 Kagome

P04 - AMAHOUCH Abdelhamid

DFT-based engineering of ferromagnetism in Cr-doped Sr1-xCrxX for spintronic applications

P05 - BATESAR Sunil

High Temperature Ultra-Low Lattice Thermal Conductivity in KCdP Half Heusler

P06 - BAU Nicolas

First-principles real-space embedding theory of the superconducting proximity effect

P07 - BEKADDOUR Abderrezak

Acoustic Phonon Effects in Scaled DG MOSFETs Above and Below 7 nm Using SchrÃ¶dingerâPoisson Formalism

P08 - BOLINO Maria De Los Angeles

Assessing electronic localization via normalized self-interaction in Quantum Espresso

P09 - BORGHI Andrea

Interplay between vibrational and electronic infrared spectrum in two-dimensional topological insulator using finite size models

P10 - BOUGHLIMA Loubna

First-Principles Study of the Spintronic Potential of the Rare-Earth-Based Half-Heusler Compound FeCeBi

P11 - BUNTING William Alexander

Phonon screening of excitons in semiconductor heterostructures

P12 - CABEZAS ESCARES Javiera Fernanda

Strong Electron-Phonon Coupling via Rigid Shifts and Reservoir Pinning

P13 - CHRAFIH Younes

Impurity Effects and Polaronic Behavior in Ni-Doped SnO_2: Bridging Experiment and First-Principles Theory

P14 - CONTANT Damian Marcin

Tight-Binding Modelling for the Phonon-Guided Generation of Hot Carriers

P15 - DAHRI Soukaina

DFT study of structural, electronic, and optical characteristics of Cs2RbAuM6 (M = Cl, F)

P16 - DAS Suvadip

Optical properties, Electron-phonon coupling and Spin fluctuations in 2D Quantum Materials

P17 - DOWLATABADI Mitra

First-Principles Wannier-BdG Modeling of Proximity-Induced Topological Superconductivity in Nb/Bi2Te3 Heterostructures

P18 - ELAPROLU Narsimha Rao

Pressure And Magnetic Field Control Of The Topological Phase In Antiferromagnetic Bilayers

P19 - FERNANDES MACHADO David

Exploring new route to boost thermoelectricity: phonon drag enhancement through interface effects

P20 - FILIPOVIC Lenka

First-Principles Analysis of Electronic Structure in Layered Phyllosilicates

P21 - GHIMIRE Amar Raj

Developing Machine Learning Force Fields for Amorphous Oxides: The Case of a-Al2O3

P22 - GOGOI Sanat Kumar

DFT+GW approach for calculating Charge Transition Levels Accurately

P23 - IQBAL Safdar

Phonon-assisted carrier transport and indirect optical absorption of cubic boron nitride from first-principles

P24 - JANA Susmita

Observation of Momentum Forbidden Γ-K Exciton in a MoS2 - CrCl3 Heterostructure

P25 - JYOTI -

Efficient Modeling of Electron-Phonon Scatterings in Low Thermal Conductivity Semiconductor BaCuGdTe3 to study Charge Transport

P26 - KLUIBENSCHEDL Florian

First-principles phonon self-energy including one-electron-two-phonon coupling

P27 - KREMEYER Laurenz

Transition from Population to Coherence-dominated Non-diffusive Thermal Transport

P28 - KUKRETI Sumit

Extraction of deformation potential and carrier scattering in Half Heusler thermoelectric materials

P29 - KURBAY Alp Umut

Rutile $Ge_xSn_{1-x}O_2$ Alloys for Ultra-Wide Bandgap Electronics: Phase Stability and Bandgap Engineering

P30 - KUSETIC Filip

Ab initio modeling of defects and polarons in Barium Titanate

P31 - LEE Jae Seong

First-principles Study on Symmetry-protected Dirac Nodal Lines in a Square Net Material CaZnBi2

P32 - LISTA Stefano

g-C6N6: A 2D Semiconductor with Dirac Cones & Flat Bands

P33 - LIU Binbin

Towards automated high-throughput electron-phonon carrier transport calculation with EPW

P34 - LOPEZ Jimena Teresa

Effect of Strain on the Superconducting Properties of Niobium

P35 - MAHEPAL Nisha Kishorbhai

Polaron-Driven Transport and Exciton–Phonon Coupling in Nitride Perovskites: A First-Principles Perspective

P36 - MEYER Sabrina Anika

Spatially Resolved Photoluminescence of Interlayer Excitons in Transition Metal Dichalcogenide Heterostructures

P37 - MISHRA Abhijeet

Pressure-Driven Enhancement of Conventional Superconductivity in Symmetry Reduced Multicomponent Hydride-Derived systems

P38 - NEDELL Jack Gillean

First-principles quasi-harmonic study of phase competition in NaNbO3

P39 - NOVOA AGUIRRE Trinidad Antonia

Non-perturbative theory of the electron-phonon coupling and its first-principles implementation

P40 - PATEL Paras Rajeshkumar

Unveiling a Phonon-Mediated Pathway for Structural Transformation in Yttrium

P41 - PATEL Shubham

Phonon self-energy correction in phonon-mediated nonlinear optical conductivity

P42 - PAUL Dwaipayan

Negative mobility and electron hole bifluidity in doped graphene

P43 - PILLAI Ashwin Anil

Phonon-assisted light absorption and emission in cubic boron nitride

P44 - PRAMANICK Subhajit

Intertwined charge density wave instability and superconductivity from electron-phonon coupling

P45 - RAJKOV Bogdan

Coupled electron-phonon hydrodynamics and Viscous Thermoelectric Equations

P46 - RANI Dimple

Strain-Driven Control of Hall Transport and Optical Absorption in Monolayer AsTeBr

P47 - RUDRA Sourav

Electron-phonon Renormalization in Momentum-resolved Electronic Structure of Scandium Nitride

P48 - SCALISE MACIEL Levy

Electron-Phonon Coupling in the Double Perovskite La2 MnNiO6 : A First-Principles FP-LAPW Study as a Starting Point for Many-Body Treatments

P49 - SEMWAL Shantanu

Concerted rattling-induced strong anharmonicity and phonon coherence lead to ultralow glasslike thermal conductivity in TlAgTe

P50 - SHABNAM Sabana

Coupling Molecular Dynamics Simulation to the Multiple Scattering Calculations : Application to the Time Resolved X-Ray Photoelectron Diffraction (TR-XPD)

P51 - SHARMA Abhiraj

Real-Space formalism for phonons within density functional perturbation theory

P52 - SIDDHARTH -

First-principles many-body study for electronic, optical, and excitonic properties of RbTlCl3 perovskite for solar cells

P53 - SINGH Zimmi

Spin-Split Phonon-Limited Carrier Mobilities from Electron-Phonon Coupling in 2D VX2Â (X = S, Se) Bipolar Magnetic Semiconductors

P54 - SINHA Priyanka

Strain induced tunable band gap and optical properties of graphene on hexagonal boron nitride

P55 - SOUROUNIS Konstantinos

Phonon-induced superconductivity in rhombohedral multilayer graphene from first principles

P56 - TEN EIKELDER Henricus Robertus Alphonsus

A New Approach to Variable-Cell Structural Relaxation of Anharmonic Crystals in Finite-Temperature and High-Pressure Conditions

P57 - TINTE MONTALBETTI Silvia Noemi

Local structural distortions, hydrogen bonding, and vacancy defects in hybrid perovskites from first-principles

P58 - TRUKHAN Elena

Dragful magnetotransport in elphbolt

P59 - URQUIZA TOLEDO Maria Laura

Probing Electron-Phonon Interaction with Resonant Inelastic X-ray Scattering

P60 - VEDANT Aaditya

Electron phonon coupling in presence of strong correlations: possible low-energy models

P61 - WANG Kang

Phonon screening of excitons in the Ruddlesden-Popper structure of SrTiO3

P62 - WINKA Nils Anders Hans

Valley differences in monolayer MoS2 calculated with the GW approximation

P01

Harnessing Linear and Nonlinear Optical Responses in Ferroelectric $LaMoN_3$ for enhanced Photovoltaic Efficiency

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Nitride perovskites represent an emerging class of functional materials with diverse predicted properties but remain underexplored due to the synthesis challenges associated with oxygen-free nitrides. Among them, $LaMoN_3$ has recently been reported as a polar, oxygen-free nitride perovskite exhibiting excellent dynamic stability and ferroelectricity under moderate pressure. However, its phase stability, optical response, and carrier dynamics under high pressure remain largely unexplored. In this work, we systematically investigate the pressure-dependent properties of $LaMoN_3$ up to 40 GPa using first-principles methods-density functional theory (DFT), density functional perturbation theory (DFPT), many-body perturbation theory (G_0W_0 and Bethe-Salpeter equation), and the tight-binding approximation (TBA). Our results reveal that $LaMoN_3$ remains dynamically stable and retains a single-phase structure throughout the investigated pressure range. The indirect bandgap decreases from 2.17 eV (0 GPa) to 1.45 eV (40 GPa) at the G_0W_0@PBE level, while the exciton binding energy reduces with pressure, enhancing the spectroscopic limited maximum efficiency (SLME). Carrier-phonon coupling, analyzed via the Fröhlich model, strengthens with pressure, leading to lower carrier mobility. Furthermore, bulk photovoltaic (BPV) and nonlinear optical responses exhibit a nonmonotonic pressure dependence, with the shift current density peaking around 15 GPa before declining at higher pressures. These findings suggest pressure as a tunable parameter for optimizing optical and photovoltaic efficiency. A multi-junction device design is proposed, integrating the 40 GPa phase for enhanced linear response and the 15 GPa phase for maximized nonlinear current, offering a synergistic route toward high-efficiency photovoltaic devices.

P02

Berry Curvature-Induced Nonlinear Transport and Optical Phenomena in Quantum Materials

P03

Symmetry-broken ground state and phonon mediated superconductivity in CsV_3Sb_5 Kagome

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The newly discovered family of non-magnetic Kagome metals AV_3Sb_5 (A=K,Rb,Cs) provides a unique platform for exploring the interplay between charge density wave (CDW) order, superconductivity, non-trivial topology, and spontaneous time-reversal symmetry breaking [1]. Although characterizing the CDW phase is essential for understanding and modeling these exotic phenomena, its nature remains unresolved. In this work, we employ first-principles free-energy calculations, accounting for both ionic kinetic energy and anharmonic effects, to resolve the atomistic phase diagram of CsV_3Sb_5 and its charge ordering structure [2]. Our results uncover that the CDW ground state is formed by reconstructed vanadium Kagome layers in a triangular-hexagonal pattern, featuring energetically degenerate different stacking orders. This accounts for the various out-of-plane modulations observed experimentally and supports the coexistence of multiple domains. The discovered symmetry-broken ground state is consistent with the absence of any electronic anisotropy in transport experiments. By combining anharmonic phonons with the calculation of electron-phonon matrix elements, we predict a superconducting critical temperature for the CDW phase in agreement with experiments, showing that superconductivity is phonon mediated. These findings not only resolve a long-standing structural puzzle, but also clarify the impact of the CDW in superconductivity, highlighting its fundamental importance in shaping the low-temperature quantum phase diagram of Kagome metals.

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P04

DFT-based engineering of ferromagnetism in Cr-doped $Sr_{1-x}Cr_xX$ for spintronic applications

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This work explores the engineering of electronic, magnetic, and elastic properties in chromium-doped strontium chalcogenides SrX (X = S, Se, Te) using ab initio calculations, accounting for the Hubbard correction (U) and strain effects. We demonstrate that Cr doping effectively engineers a robust half-metallic character and stabilizes a ferromagnetic ground state, with spin polarization reaching 100% in most configurations. The engineered ferromagnetic phase is thermodynamically and magnetically stable, as confirmed by negative formation energies and Curie temperatures well above room temperature, reaching 464 K, 475 K, and 570 K for SrS, SrSe, and SrTe, respectively, at a Cr concentration of 24%. Strain engineering (2% and 4%) provides an additional degree of control over the electronic structure, leading to noticeable shifts in the density of states and band-gap reduction, while simultaneously strengthening magnetic interactions and preserving half-metallicity. From a mechanical engineering perspective, Cr-doped SrS exhibits high elastic moduli, making it suitable for mechanically robust spintronic devices and spin filters. Cr-doped SrSe offers a balanced combination of strength and ductility, making it promising for magnetic tunnel junctions in MRAM technologies. Meanwhile, Cr-doped SrTe shows enhanced ductility and deformability, enabling flexible spintronic devices such as SpinFETs. Overall, this study highlights how chemical doping and strain engineering can be employed to tailor ferromagnetism and mechanical properties, positioning Cr-doped SrX compounds as versatile candidates for next-generation spintronic applications.

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P05

Abstract

High Temperature Ultra-Low Lattice Thermal Conductivity in KCdP Half Heusler

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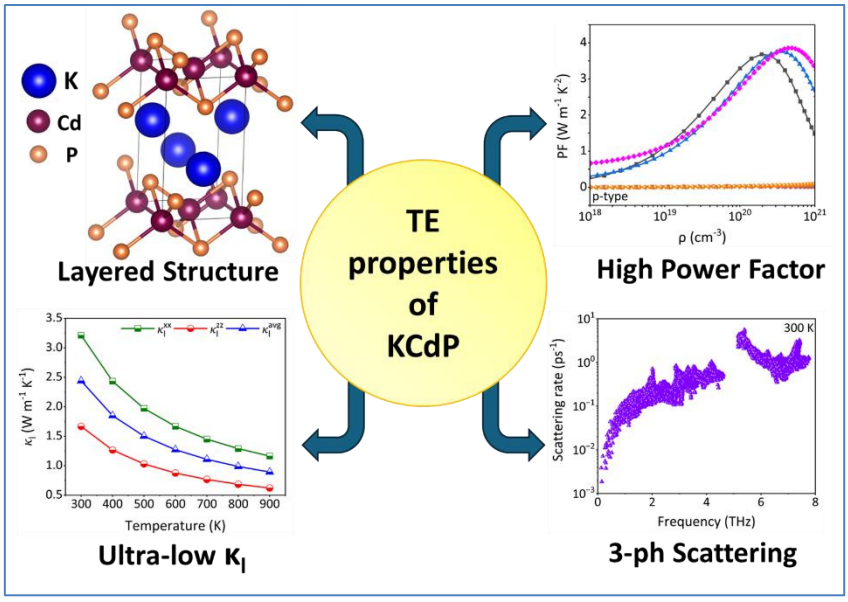
Thermoelectric materials could help turn waste heat into electricity, but their efficiency is often limited by low ZT values. Here, we present a comprehensive computational investigation of KCdP, a quasi-two-dimensional layered compound, leveraging first-principles calculations and Boltzmann transport theory to unravel its thermoelectric potential. Structural and mechanical analyses reveal KCdP's ductile nature, underpinned by mixed ionic-covalent bonding, while electronic structure studies highlight anisotropic conduction with multi-valley valence band maxima-features conducive to high Seebeck coefficients and electrical conductivity. Phonon transport calculations, incorporating three-phonon scattering and wave-like tunneling effects, demonstrate exceptionally low lattice thermal conductivity (~0.89 W m^{-1} K^{-1} at 900 K), driven by strong anharmonicity evidenced by large Gr¨uneisen parameters. Carrier relaxation time analysis further confirms favorable charge transport properties under p-type doping. Remarkably, KCdP achieves a ZT exceeding 1.0 in the intermediate-temperature regime, positioning it as a compelling candidate for efficient thermoelectric energy conversion. This work underscores the potential of engineered quasi-2D materials to bridge the gap between theoretical promise and practical applications in waste-heat recovery technologies. KCdP exhibits pronounced anisotropy in thermoelectric performance, achieving maximum efficiencies of 20.24% and 2.38% for p-type doping and 6.34% and 2.27% for n-type doping along the x and z directions, respectively, highlighting the crucial role of crystallographic orientation in device optimization.



P06

First-principles real-space embedding theory of the superconducting proximity effect

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When a superconductor is placed in contact with a normal material, Cooper pairs penetrate the latter and induce superconductivity via the proximity effect [1, 2]. Despite its central role in quantum materials, superconducting devices and topological platforms, a predictive first-principles description of the proximity effect at realistic interfaces has remained computationally prohibitive so far. Here, we fill this gap by developing a Green's-function framework based on real-space dynamical embedding that enables first-principles simulations of superconducting proximity in mesoscopic systems [3]. We show that the proximity effect admits a transparent diagrammatic formulation in terms of normal and anomalous embedding self-energies, which disentangle and quantify the distinct renormalization mechanisms generated by coupling to a superconducting bath. By combining this formalism with recursive schemes [4, 5], we compute local spectral functions and proximity lengths extending over hundreds of nanometers into the bulk without resorting to thick interface slabs. We deploy the approach on tight-binding models (Qi-Hughes-Zhang [6] and Fu-Kane-Mele [7]), where we analyze mixed-parity superconductivity in topological insulators proximitized by s-wave superconductors, and on first-principles simulations of $NbSe_2/CrBr_3$ heterostructures [8] based on density-functional theory and maximally-localized Wannier functions. Our work provides a scalable and conceptually unified framework that bridges microscopic electronic structure and mesoscale proximity physics, enabling predictive atomistic simulations of superconducting interfaces.

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P07

Acoustic Phonon Effects in Scaled DG MOSFETs Above and Below 7 nm Using Schrödinger–Poisson Formalism

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Poster Description and abstract

The continuous downscaling of CMOS technologies has led Double-Gate (DG) MOSFETs to channel lengths in the nanometric and sub-7 nm regime, where quantum confinement and scattering mechanisms play a dominant role in carrier transport. Among these mechanisms, acoustic phonon scattering remains a fundamental limiting factor for carrier mobility and energy dissipation, even at room temperature. Understanding its impact across different scaling regimes is therefore essential for both device performance optimization and energy-aware modelling.

In this work, we investigate the effect of acoustic phonon scattering in nanometric DG MOSFETs by distinguishing two channel length regimes : devices with channel lengths above 7 nm and ultra-scaled devices with channel lengths below 7 nm. This separation allows a clear identification of the transition from quasi-classical transport to strongly quantum-confined transport, where wavefunction localization and subband occupation significantly modify carrier–phonon interactions.

The study is performed at a temperature of 300 K using a self-consistent Schrödinger–Poisson modelling framework developed during my doctoral research. The model explicitly accounts for two-dimensional acoustic phonon scattering and captures quantum confinement effects in the channel. For each channel length regime, electrical characteristics are simulated under identical biasing conditions to ensure a meaningful comparison.

A particular emphasis is placed on the extraction of phonon-limited mobility, which serves as a key metric to quantify transport degradation induced by acoustic phonons. The results highlight how channel length scaling influences mobility behavior, revealing a pronounced reduction in the sub-7 nm regime due to enhanced confinement and increased scattering rates. In contrast, devices with channel lengths above 7 nm exhibit mobility trends closer to classical expectations.

These findings provide valuable physical insight into the role of acoustic phonons in scaled DG MOSFETs and contribute to a better understanding of performance limits and energy dissipation in ultra-scaled devices. The presented analysis also lays the groundwork for future extensions of the model to include optical phonon scattering, which is expected to become increasingly relevant under high-field and high-energy operating conditions.

P08

Assessing electronic localization via normalized self-interaction in Quantum Espresso

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Density functional theory (DFT) is one of the most widely used methods for first-principles (*ab initio*) calculations in condensed matter and molecular systems, and has proven highly successful in predicting material properties in close agreement with experimental observations [1]. Among these, the degree of electronic localization is particularly important in disordered systems, such as defected crystals and amorphous materials, and it plays a central role in the study of insulators, metals, and semiconductors [2].

In the materials science and chemistry communities, several tools are commonly used to analyze electronic localization based on the electron density, including the electron localization function (ELF) and the inverse participation ratio (IPR) [3]. These approaches are typically implemented as post-processing techniques within the DFT framework to quantify localization on a given scale. However, methods such as the IPR often require additional data processing steps, such as the generation of real-space electronic density files, which increases both computational cost and analysis complexity.

In this context, we propose a method to characterize localized states in crystalline materials and amorphous semiconductors based on the self-interaction (SI) contribution to the Hartree energy within DFT. Self-interaction remains in the Hartree term due to the use of the total electronic density in self-consistent field calculations, and it refers to the unphysical interaction of an electron with itself in a periodic system. This contribution increases for localized states, while remaining minimal for extended (bulk-like) states. By normalizing the SI of a given state with respect to that of a bulk reference state, we define a dimensionless parameter that quantifies localization: values close to 1 correspond to fully delocalized states, whereas values greater than 1 indicate increasing localization [4]. A key advantage of this approach is its orbital-level description, which enables a detailed analysis of localization across different material phases, particularly near the band edges.

In this work, we present an efficient and scalable implementation of the normalized SI method within the Quantum ESPRESSO framework. We demonstrate its performance through simulations of isolated vacancies, divacancies, and amorphous systems using supercells containing up to 998 atoms, and we evaluate convergence with respect to supercell size in large-scale DFT calculations. Additionally, we examine vacancy–vacancy interactions to gain insight into defect clustering mechanisms. This implementation provides a practical and accessible tool for identifying localized states, significantly reducing the effort required for subsequent electronic structure analyses.

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P09

Abstract template for 2026 School on Electron-Phonon Physics and Many-body Perturbation Theory

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Recent studies proposed a new approach to study the topological phase transitions, based on the assessment of the vibrational resonances in the infrared spectrum [1]. Specifically, within the Haldane model —a prototypical 2D topological insulator— the Born effective charges, quantifying the intensity of vibrational resonances, exhibit a discontinuous jump at the topological phase transition. This result is obtained by exploiting the connection between the electronic and vibrational responses at the band edges [2].

The effects of the metallic edge states on the infrared response in topologically non trivial states of the Haldane model are addressed using two different 2D systems: a finite size model with open boundary conditions [3][4], and a ribbon with a single periodic direction. In both cases the value of the Born effective charges differs from the one obtained in the infinite crystal only near the surface, remaining always finite; this surface effect decays exponentially inside the system, where the Born effective charges match the behaviour seen in periodic system. In the ribbon, the longitudinal electronic conductivity along the period direction displays the signature of a Drude peak, due the presence of the metallic surface states in the topological phase. Nevertheless, the metallic states does not compromise the visibility of the vibrational fingerprints on the full infrared absorption spectrum, confirming their role as a probe for the topological phase also for real finite system.

For instance, the result of this work could provide alternative method based on the optical response for studying the properties of topologically nontrivial Germanane nanoribbons [5].

ACKNOWLEDGMENTS

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P10

First-Principles Study of the Spintronic Potential of the Rare-Earth-Based Half-Heusler Compound FeCeBi

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Abstract

Systematic theoretical research of the half-Heusler compound FeCeBi was carried out using first-principles calculations on density functional theory (DFT) here. Three candidate crystal structures were studied; of which it was found that the ground-state most stable configuration was the α-phase in the ferromagnetic (FM) state. Electronic band structure computations verified that FeCeBi is an ideal half-metal with a semiconducting gap in the spin-up channel and metallic behavior in the spin-down channel and hence it is highly potential for spintronic devices. Elastic properties such as elastic constants (C_{11}, C_{12}, C_{44}) confirmed mechanical stability based on Born-Huang criteria. Other mechanical indicators such as the ratio B/G and Poisson's ratio indicated a good balance of ductility and stiffness. Additionally, the electronic structure was determined to be structurally deformed sensitive; when compressed, the band gap expands, while it reduces with dilatation. This tunability makes it easy to adapt FeCeBi to specific applications. Optical study revealed spin-dependent effects, further confirming the compound's asymmetric half-metallic character. Generally, the results demonstrate that FeCeBi is a very suitable material candidate for future spintronic and multifunctional device technologies.

Keywords: *Half-Heusler FeCeBi; Mechanical properties; Dilatation and compression; Optical properties; Thermodynamic properties.*

P11

Phonon screening of excitons in semiconductor heterostructures

P12

Strong Electron-Phonon Coupling via Rigid Shifts and Reservoir Pinning

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We study the MgB_2-derived two-dimensional superconductor H–MgB_2 [1] as a *gedanken-experiment* designed to isolate pairing mechanisms that differ from those of bulk MgB_2. This system provides a controlled computational testbed to identify transferable physical principles that may emerge in chemically stable 2D materials.

Using first-principles calculations, we show that strong electron–phonon coupling is dominated by zone-center (Γ-point) phonons that conserve crystal momentum. Rather than driving a nesting-induced instability, these modes enhance coupling through two key effects: (i) they break the equivalence between M and M', splitting the Van Hove singularity via anisotropic hopping renormalization; and (ii) they produce rigid-like shifts of bands near the Fermi level without generating new hybridized states. As a result, the overall Fermi-surface connectivity is preserved, with no Brillouin-zone folding or Fermi-surface reconstruction.

To rationalize these trends, we develop a minimal tight-binding model capturing the interplay between charge transfer and electronic reordering, and benchmark it against DFT. The combined action of phonon-driven vHS splitting and phonon-assisted band filling provides a coherent microscopic picture for robust coupling in this simplified 2D platform.

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P13

Impurity Effects and Polaronic Behavior in Ni-Doped SnO_2: Bridging Experiment and First-Principles Theory

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We investigated the effect of nickel (Ni) doping on the structural, morphological, and optoelectronic properties of SnO_2, combining experimental characterization and first-principles simulations. Ni was incorporated at concentrations of 1%, 2%, 3%, 4%, and 5% to systematically probe its role as an impurity in the SnO_2 lattice. Experimentally, X-ray diffraction and electron microscopy revealed modifications in crystallite size and surface morphology with increasing Ni content. Optical measurements indicated changes in the band gap and absorption properties, suggesting tuning of electronic states by Ni incorporation. These experimental results were validated and interpreted through density functional theory (DFT) calculations, which provided insights into the formation energies, electronic density of states, and potential polaronic effects induced by Ni impurities. Our combined approach elucidates how controlled Ni doping modulates the electronic structure and optoelectronic performance of SnO_2, offering guidance for designing oxide-based functional materials for applications such as electron transport layers in photovoltaic devices.

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P14

Tight-Binding Modelling for the Phonon-Guided Generation of Hot Carriers

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In the field of photocatalysis, metallic nanoparticles (NPs) stand as ideal candidates to induce chemical reactions in molecular adsorbates [1]. A direct illumination at specific frequencies generates plasmons on the NP surface. Their decay can then lead to the formation of hot electrons and/or hot holes under the Landau damping process, which, when transferred to the adsorbates, modifies the activation profiles [2, 3].
Another non-radiative decay pathway involves the vibrational excitation of the NP phonon modes. While this process is usually perceived as a cause of energy loss, it can also lead to a vibrational transfer to the adsorbate, thus potentially opening different reaction routes. To model these phonon-guided processes, we need to describe electron-phonon interactions within the metallic NPs.
In this work, we seek to perform a tight-binding parametrization of the electronic band structure for systems featuring small atomic displacements away from equilibrium, in order to obtain a description of electron-phonon coupling [4]. We will present the fitting of the Slater-Koster parameters to density functional theory calculations for non-ideal bulk structures such as strained crystals, and the validation of whether such Hamiltonians can accurately describe electron-phonon coupling.

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P15

DFT study of structural, electronic, and optical characteristics of Cs_2RbAuM_6 (M = Cl, F)

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Abstract

Using density functional theory (DFT), this study investigates the structural, electronic, optical, and thermoelectric properties of halide double perovskites Cs_2RbAuX_6 (X = Cl, F). The aim is to assess the viability of these materials for next-generation optoelectronic and energy applications and to elucidate the influence of halogen substitution on their multifunctional behavior. Structural stability was verified using the Birch-Murnaghan equation of state combined with total energy minimization. Electronic band structure calculations reveal spin-polarized semiconducting behavior, with halogen choice significantly affecting band gaps. Optical studies demonstrate strong ultraviolet absorption, particularly in $Cs_2RbAuCl_6$, suggesting potential use in UV detectors. Thermoelectric analysis indicates that Cs_2RbAuF_6 exhibits a higher Seebeck coefficient and figure of merit (ZT), highlighting its promise for thermal energy harvesting. These results underscore the tunability of these materials for tailored applications.

Keywords: DFT; Spin-polarized semiconductor; Electronic properties; Optical properties; Thermoelectric properties.

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P16

Optical properties, Electron-phonon coupling and Spin fluctuations in 2D Quantum Materials

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Abstract

Two-dimensional quantum materials such as $MoSe_2$, and other transition metal dichalcogenides (TMDs) are reputed for atomically thin spintronic, valleytronic and quantum spin Hall devices. With the advent of quantum computing and superconducting devices, an exploration into the topological manifestation in 2D materials have been deemed indispensable. Functional two-dimensional materials are promising for advanced atomically thin electronic and optoelectronic devices, such as light emitting diodes (LEDs), ultrathin solar cells, and valleytronic devices. Recently, atomic layers of α-PbO and hexagonal Si/Ge have been successfully grown using micromechanical and sonochemical exfoliation. We performed first-principles calculations based on density functional theory and many-body perturbation theory to investigate the electronic and optical properties (utilizing the GW and BSE methodology) of monolayer, bilayer, and bulk litharge α-PbO. Further, we have investigated the phonon lifetimes and linewidths, Gruneisen parameters and Raman modes in layered hexagonal phases of Si/Ge . A latest addition to the landscape of exotic 2D materials pertains to the discovery of not yet foretold superconducting state in monolayers of $NbSe_2$ dubbed 'Ising superconductivity'. In our study, we have investigated the energetics, magnetic moment and fully q-dependent spin susceptibility in order to pin point the location of the ferromagnetic instability in the Brillouin Zone of this material. This involves our methodology of inverting the random-phase approximation, and utilization of first principles calculations artificially stabilized by Hubbard interactions and spin-spiral calculations for evaluation of the fluctuation renormalized spin susceptibility. Finally the role of spin fluctuations and electron phonon coupling in determining the superconducting order parameter for the newly popular 2D Ising superconductor $NbSe_2$ will be discussed.

P17

First-Principles Wannier–BdG Modeling of Proximity-Induced Topological Superconductivity in Nb/Bi_2Te_3 Heterostructures

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We present a first-principles study of the superconducting proximity effect in Nb/Bi_2Te_3 heterostructures. Using a Wannier-based Bogoliubov–de Gennes framework, with electronic structure from density functional theory and pairing in Nb from Migdal–Eliashberg theory, we solve the heterostructure self-consistently at finite temperature and compute temperature-dependent superconducting properties, including the critical temperature. Regions far from the interface are treated as semi-infinite through embedding potentials to reduce finite-size effects. After validating the method for bulk Nb, we analyze the singlet and triplet anomalous densities induced in the topological insulator, providing microscopic insight into proximity-induced superconductivity.

P18

Pressure And Magnetic Field Control Of The Topological Phase In Antiferromagnetic Bilayers

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Antiferromagnetic bilayers are said to be A-type when spins align ferromagnetically within each layer but point in opposite directions in the two layers, resulting in a zero net magnetization. The opposite orientation of majority spins in the two layers strongly suppresses interlayer hopping and the electronic structure is not affected significantly by a change in interlayer distance. Nonetheless, an external magnetic field can drive a metamagnetic transition into a fully ferromagnetic state, where spins in both layers are parallel, so that interlayer hopping is possible and energy bands are sensitive to the separation between the layers. This difference can be exploited to manipulate the energy bands of an A-type antiferromagnetic bilayer by means of the combined effect of pressure and magnetic field. Here we consider bilayer CrSBr as a prototypical example and show using first-principles simulations that pressure affects the interlayer distance, enhancing the interlayer hopping in the ferromagnetic state, and eventually closes the energy gap, inducing a topological phase transition. Remarkably, depending on the magnetization direction it is possible to tune the system either in a quantum anomalous Hall insulating state when spins are out-of-plane or into a half Chern-Weyl semimetallic phase when spins are in-plane, with the emergence in both cases of topological edge states. We expect this phenomenon to be general to A-type antiferromagnetic bilayers, opening interesting perspectives on the manipulation of their topological character towards applications in spintronics and quantum computation.

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P19

Exploring new route to boost thermoelectricity: phonon drag enhancement through interface effects

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Our theoretical project aims at opening new ways to improve the thermoelectric efficiency of materials, by exploring the phonon drag effect, which arises from the momentum transfer (or drag) between the out-of-equilibrium phonon and electron populations, and which is responsible for the strong increase in Seebeck and Peltier coefficients of thermoelectric materials at low temperature.

In this poster, we present our recent theoretical work on the phonon-drag effect in silicon nanostructures [1]. We then discuss how the presence of a substrate can shift the temperature range in which the phonon-drag contribution becomes significant. To support this idea, we present experimental findings that corroborate this behavior [2].

Motivated by these observations, our ultimate goal is to develop a numerical framework capable of describing the coupled transport of charge and heat carriers at the interface between a conducting system and a substrate acting as a phonon bath, with particular emphasis on the phonon-drag effect. In this poster session, we present our main preliminary theoretical results.

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P20

First-Principles Analysis of Electronic Structure in Layered Phyllosilicates

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Naturally occurring phyllosilicates such as talc and kaolinite-type minerals constitute an important class of intrinsic layered materials and can be regarded as natural analogues of two-dimensional (2D) systems. Owing to their sheet-like crystal architecture, these materials exhibit strong in-plane bonding and direction-dependent physical properties, making them attractive platforms for studying low-dimensional behavior in naturally occurring compounds.

The crystal structures of phyllosilicates are built from tetrahedral (T) sheets composed of SiO_4 units and octahedral (O) sheets containing metal-centered octahedra. In kaolinite-type minerals, individual layers consist of a single tetrahedral sheet bonded to an octahedral sheet (T–O), whereas talc adopts a 2:1 layered structure in which an octahedral sheet is sandwiched between two tetrahedral sheets (T–O–T) [1]. These distinct stacking motifs lead to different interlayer bonding mechanisms and govern the degree of coupling between adjacent layers.

In this work, we investigate the electronic properties of layered phyllosilicates, focusing primarily on talc and kaolinite-type minerals. The calculated electronic band structures reveal wide band gaps at the PBE level and a strong dependence of band dispersion on the layered crystal architecture. Differences between talc and kaolinite-type minerals arise from their distinct stacking arrangements and interlayer interactions, which directly influence electronic anisotropy and interlayer coupling.

First-principles calculations were carried out using the Quantum ESPRESSO package [2], based on density functional theory with plane-wave basis sets and ultrasoft pseudopotentials. Exchange–correlation interactions were treated using the PBE generalized gradient approximation, and Grimme-D2 van der Waals corrections were included to properly account for interlayer interactions.

These results provide fundamental insight into how naturally occurring layered silicates behave at the electronic-structure level. Their intrinsic two-dimensional building blocks, combined with structural diversity and tunable electronic characteristics through defects, doping, or layer engineering, make talc and kaolinite-type minerals promising candidates for use in van der Waals heterostructures, dielectric layers, and as substrates for two-dimensional electronic and optoelectronic systems. More broadly, this study establishes naturally layered phyllosilicates as a versatile platform for exploring structure–property relationships in low-dimensional materials.

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P21

Developing Machine Learning Force Fields for Amorphous Oxides: The Case of a-Al2O3

P22

DFT+GW approach for calculating Charge Transition Levels Accurately

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Using a combined density functional theory (DFT) and GW formalism, we study the electronic structure and charge transition levels (CTLs) of oxygen vacancy defects in m-ZrO_2. The CTLs are calculated using two paths and employing electrostatic corrections due to localized charge at the defect site. We find +1/0 CTL is at 3.48 eV (2.50 eV) and +2/+1 CTL is at 1.92 eV (0.98 eV) for 3-fold (4-fold) oxygen vacancy in m-ZrO_2. We also describe a relaxation mechanism of atoms near an oxygen vacancy site. Finally, we compare the calculated CTLs using only density functional theory and the combined approach of both density functional theory and GW method with appropriate electrostatic corrections. Our results agree well with the experimental findings of electronic trap level in m-ZrO2

P23

Phonon-assisted carrier transport and indirect optical absorption of cubic boron nitride from first-principles

P24

Observation of Momentum Forbidden Γ-K Exciton in a MoS_2 - $CrCl_3$ Heterostructure

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Hybrid excitons in a type-II magnetic-nonmagnetic van der Waals heterostructure are the foundation to examine magnetic proximity interactions leading to significant interlayer coupling and emergent quasiparticles in these materials. Such excitons are being observed at a lower energy spectrum than their constituent parent materials due to electronic band offset and magnetism induced high coulomb interaction. Here we are presenting nontrivial approach to observe momentum forbidden Γ-K hybrid exciton with comparable PL intensity in a planar magnetic substrate and MoS_2 monolayer. We have thoroughly investigated the role of band hybridization involved in this process. The optical hybridization opens a new way by modifying the spin textures and breaking the symmetry at the interface which will offer a gateway for this material to use in various spin and optoelectronic devices. We found zero polarization of this Γ-K hybrid exciton contributing to the involvement of Γ and K valley and extended lifetime of this exciton provide validation towards its momentum dark nature. Further through the lifetime calculations, we have demonstrated that this newly formed state is the energetically most favourable state than the conventional K-K exciton. This interfacial engineering approach facilitates a new degree of control for studying correlated excitonic phenomenon in two dimensional heterostructures.

P25

Efficient Modeling of Electron–Phonon Scatterings in Low Thermal Conductivity Semiconductor $BaCuGdTe_3$ to study Charge Transport

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Thermoelectric materials have great potential to mitigate environmental damage by converting the wasted heat generated from fossil fuel combustion into electrical energy [1]. Their efficiency depends on achieving high electrical conductivity while minimizing phononic transport. The occurrence of low phonon transport and high electrical transport is a rare phenomenon in crystalline semiconductors [2]. In this work, using first-principles density functional theory calculations, Boltzmann transport theory and explicit consideration of phonon-phonon and electron-phonon interactions, we study $BaCuGdTe_3$, a layered quaternary chalcogenide semiconductor, which exhibits high electrical transport properties and exceptionally low lattice thermal conductivity [3].

While studying the electron-phonon interactions, the fully iterative solution becomes computationally expensive due to the requirement of very dense momentum grids, especially for such large systems with 12 atoms in the unit cell. Even with the use of maximally localized Wannier functions, such large systems have not yet been widely reported [4, 5]. Therefore, to gain physical insight into the electron–phonon interaction, we used models for the relevant scattering mechanisms, in which the electron–phonon matrix elements depend only on intrinsic material properties [6]. We separately considered acoustic deformation potential scattering, piezoelectric scattering, polar optical phonon scattering, and ionized impurity scattering. The total scattering rates were then obtained using Matthiessen's rule and used to calculate the electronic transport properties. We showed that this compound has excellent electrical transport properties due to strong covalent bonding within its layers. Along with that $BaCuGdTe_3$ show ultralow lattice thermal conductivity due to the layered structure and local distortions present in the compound that strongly suppress acoustic phonon modes, reducing phonon group velocities and enhancing phonon scattering rates. These characteristics make $BaCuGdTe_3$ a highly promising candidate for thermoelectric applications with a high figure of merit at modest carrier concentrations and temperatures.

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P26

First-principles phonon self-energy including one-electron-two-phonon coupling

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We derive the phonon self-energy including both one-electron–one-phonon and one-electron–two-phonon interaction vertices, with all couplings obtained from first-principles calculations. The full self-energy matrix, including off-diagonal terms, is computed and evaluated on-shell. We find that the two-phonon contribution grows with temperature and significantly affects the phonon renormalization at high temperatures. Results for LiF and CsPbBr3 demonstrate the quantitative impact of the two-phonon processes on phonon energies and linewidths.

P27

Transition from Population to Coherence-dominated Non-diffusive Thermal Transport

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Deviations from diffusive heat transport in high thermal conductivity crystalline insulators are generally understood within the framework of the phonon Boltzmann Transport Equation. However, for low thermal conductivity materials with large primitive cells or strong anharmonicity, the recently developed Wigner Transport Equation is more appropriate as it includes tunnelling between overlapping phonon bands. In this work, via solutions to the Wigner Transport Equation, we develop a scheme to obtain the dynamics of the phonon populations and coherences as a function of an arbitrary heat source. The approach is applied to predict size effects and dynamical thermal conductivities in $CsPbBr_3$ and $La_2Zr_2O_7$ using first-principles data as input. We predict significant deviations from the bulk thermal conductivity in these materials at length scales on the order of hundreds of nanometers to a few microns at room temperature, well within the reach of direct observation using current experimental techniques.

P28

Extraction of deformation potential and carrier scattering in Half Heusler thermoelectric materials

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The thermoelectric transport properties of materials are governed by electron–phonon scattering, including both polar and nonpolar interactions, as well as electron scattering from ionized impurities. Using the EPW formalism, we computed the electron–phonon coupling matrix elements for several half-Heusler compounds and extracted the deformation potentials associated with acoustic and nonpolar scattering mechanisms. Furthermore, employing an advanced Boltzmann transport solver as implemented in ElecTra [1], which explicitly accounts for electronic scattering arising from all relevant phonon modes and ionized impurities, we calculated their Seebeck coefficient, electrical conductivity, and power factor [2]. In addition, we are developing an approach to extract deformation potentials for doped and alloyed systems using EPW. This methodology, when integrated within ElecTra, enables the prediction of thermoelectric transport properties in experimentally realizable doped materials while significantly reducing the computational cost compared to fully first-principles transport calculations. We believe the school will provide substantial help to the aims of our project.

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P29

Rutile $Ge_xSn_{1-x}O_2$ Alloys for Ultra-Wide Bandgap Electronics: Phase Stability and Bandgap Engineering

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$Ge_xSn_{1-x}O_2$ alloys have recently attracted attention as candidate ultra-wide bandgap (UWBG) materials for power electronics due to their predicted ambipolar dopability, high carrier mobilities, and high thermal conductivity. Experiments show that these alloys can be grown as thin films over a wide composition range, have carrier mobilities that are insensitive to alloy disorder at low Ge content, and exhibit breakdown fields as high as 7.0 ± 1.4 MV/cm [1]. In this study, we perform a comprehensive investigation of the thermodynamic stability, structural parameters, and electronic properties of $Ge_xSn_{1-x}O_2$ alloys using first-principles atomistic calculations. Our thermodynamic calculations show that these alloys can be approximated as random solid solutions across all compositions; we also demonstrate that coherency strain during epitaxial growth substantially alters phase stability, suppressing the miscibility gap and critical temperature, consistent with the high solubilities observed experimentally. Calculated lattice parameters exhibit a nearly linear dependence on composition, consistent with Vegard's law and experimental measurements. We find a direct band gap at the Γ-point ranging from ~3.6 eV in SnO_2 to ~4.7 eV in GeO_2, with strong compositional bowing and light carrier effective masses. The calculated bandgaps in the Sn-rich region show a ~200 meV difference between thin films and bulk alloys, and we explore possible causes such as compressive strain and interfacial effects from the substrates. The band dispersions and anisotropic carrier effective masses provide key inputs for future first-principles electron–phonon coupling and carrier transport calculations using Wannier interpolation methods. Optical absorption results for the 50% alloy reveal that local alloy disorder relaxes the dipole-forbidden character of the fundamental gaps in the binaries with polarization-dependent transition strength. Our results reveal the thermodynamic origin of the metastability of $Ge_xSn_{1-x}O_2$ thin films and highlight their potential for ultra-wide-bandgap optoelectronics and power electronics applications [2].

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P30

Ab initio modeling of defects and polarons in Barium Titanate

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Ferroelectric oxides, such as lithium niobate (LNO) or barium titanate (BTO), are excellent candidates as building blocks of electro-optic modulators based on the Pockels effect due to their large electro-optic (EO) response. For a given material, the latter describes the change in refractive index with respect to the magnitude of the electric field applied to it. Hence, in the case of a strong EO response, the distance required for the phase of an optical signal to be modulated becomes shorter. While LNO is the current industrial standard, BTO exhibits a much larger Pockels effect, $\sim$ 1000 pm/V [1] vs. $\sim$ 30 pm/V for LNO. However, the EO response of BTO can be significantly altered by crystal imperfections, e.g., defects or impurities. To the best of our knowledge, no comprehensive study has been carried out to elucidate the impact of different defects on the EO performance of BTO and similar materials.

In this work, we fill this gap by comparing photoluminescence measurements of BTO samples with *ab initio* calculations of atomic structures containing various types of defects. Information about the band gap and in-gap optical transitions of the materials examined can be derived from the photoluminescence measurements. These optical transitions can then be correlated with the presence of different defects and possibly polaron states. Existing studies have mainly focused on cathodoluminescence measurements of BTO ceramic powders, which differ from our experiments in both the material composition and the measured energy range. As epitaxial BTO thin films, not ceramic powders, are of practical interest to design electro-optic modulators, we have developed a reference model to explain the optical transitions of this specific material. Our approach relies on density functional theory (DFT), as implemented in the *Quantum Espresso* package, to first create atomic systems with defects, e.g., oxygen or barium vacancies, and then compute their electronic bandstructure and optical transition energies as functions of the defect formation energies and charge state. The analysis has been expanded by also considering the presence of polarons through electron-phonon interactions using the *EPW* software. One of our major objectives consists of shedding light on the polaron properties in BTO, in particular, on their formation energy, relative position with respect to the band edges, and displacements. Next, we will determine the Pockels response of the optimized structures including both defects and polarons. This will pave the way for a better understanding of these effects on the EO response of BTO.

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P31

First-principles Study on Symmetry-protected Dirac Nodal Lines in a Square Net Material $CaZnBi_2$

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We investigate the atomic and electronic structures of $AZnBi_2$ (A = Ca, Sr, Ba) family of material using first-principles density functional theory. The material class shows interesting band structures around the Fermi energy, mainly derived from the Bi-square net. Moreover, as the A-site cation radius increases, the space group of the ground-state atomic structure changes from *P4/nmm* to *I4/mmm* space group, with associated changes in the A-site coordination around the Bi square net. Focusing on the evolution of the band structures due to the change in A-site coordination, we find that in the absence of spin-orbit coupling, either Dirac point or nodal line structures emerge along the Γ-M high symmetry line, which in turn are gapped by spin-orbit coupling. In contrast, the degeneracy at the X-point is protected by the non-symmorphic symmetry of the *P4/nmm* structure, even in the presence of the spin-orbit coupling, enforcing the semimetal phase. Our work shows the role of the symmetry that dictates the band crossings around the Fermi energy and protects the metallic phase for the *P4/nmm* structure with non-symmorphic symmetry, which is determined by the A-site coordination around the Bi square net

P32

g-C_6N_6: A 2D Semiconductor with Dirac Cones & Flat Bands

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The ongoing search for two-dimensional (2D) materials often aims to combine the exceptional charge carrier mobility of graphene with a finite bandgap, a crucial requirement for novel electronic and optoelectronic applications. This work presents a comprehensive first-principles study of g-C_6N_6 (graphitic heptazine-based carbon nitride), a 2D organic direct-gap semiconductor characterized by a porous Kagome-like lattice geometry. Through a rigorous computational approach combining Density Functional Theory (DFT), Density Functional Perturbation Theory (DFPT), and the Boltzmann Transport Equation (BTE), we investigate the structural, electronic, optical, vibrational, and transport properties of this material.
Our electronic structure calculations reveal that g-C_6N_6 exhibits a direct bandgap at the K point of the Brillouin zone. Remarkably, the band structure hosts both highly dispersive Dirac cones in the conduction band (ensuring high carrier mobility) and nearly flat bands in the valence region, which promote electronic localization and strong many-body correlations. Optical property analysis using a scissor operator on the energy spectra based on the work of Liang et al. within an independent particle approach, supplemented by the Ritova-Keldysh potential model, uncovers an exceptionally large exciton binding energy of 2.96 eV.
Furthermore, phonon dispersion calculations confirm the dynamical stability of the 2D lattice, with electron-phonon coupling found to be most intense for high-energy optical phonons. We investigate the intrinsic charge transport and ultrafast dynamics by evaluating band-projected scattering rates. Transport calculations indicate that carrier mobility at the Dirac cones reaches high values and is heavily dominated by acoustic phonon scattering. In stark contrast, mobility at the band edges (Conduction Band Minimum and Valence Band Maximum) is significantly suppressed. Consequently, at room temperature (300 K), carrier relaxation times at the band edges are drastically reduced to the order of a few femtoseconds. These findings establish g-C_6N_6 as a highly promising platform for exploring the interplay between high charge mobility and correlated quantum phases in 2D polymers.

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P33

Towards automated high-throughput electron-phonon carrier transport calculation with EPW

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The accurate prediction of charge carrier mobility is crucial for the design and discovery of next-generation electronic and optoelectronic materials. First-principles calculations based on the Boltzmann transport equation (BTE) and dense electron-phonon (e-ph) matrix elements provide predictive accuracy but are notoriously complex to execute. They require meticulous orchestration of ground-state calculations, phonon dispersions, robust Wannierization, and handling of long-range interactions, making them highly resistant to high-throughput (HT) screening. In this work, we present a fully automated, robust framework for computing e-ph transport properties using the EPW code, implemented within the AiiDA materials informatics infrastructure. Our framework breaks down the complexity into modular AiiDA workchains: an EpwPrepWorkChain that automates coarse-grid electron and phonon calculations along with automatic Wannier function generation using Wannier90; a QuadrupoleWorkChain that seamlessly handles dynamical quadrupoles for accurate long-range corrections in polar materials; and a MobilityWorkChain that executes convergence-controlled calculations of carrier mobility using both the self-energy relaxation time approximation (SERTA) and the iterative BTE (iBTE). We demonstrate the robustness and efficiency of this automated approach on a test set of materials, showcasing its capability to manage complex execution graphs and ensure data provenance. This framework paves the way for routine high-throughput screening of transport properties across large materials databases.

P34

Effect of Strain on the Superconducting Properties of Niobium

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Niobium is a well known conventional type-I superconductor and a useful reference system for studying electron-phonon physics. One particularly relevant feature is the Kohn anomaly in its phonon spectrum [1], which reflects strong coupling between specific phonon modes and the electronic states near the Fermi level. While the effects of pressure and doping in Nb have been explored in detail [2], the impact of anisotropic strain is still not as systematically established, even though strain is an experimentally accessible way to tune lattice geometry and symmetry.

Our study is based on first-principles calculations within Density Functional Theory, combined with phonon calculations and Density Functional Perturbation Theory. Starting from the equilibrium BCC structure, controlled tensile and compressive strain are applied to the lattice, and the resulting changes in band structure, density of states at the Fermi level, phonon spectra, and Fermi-surface topology are analyzed, with particular attention to the evolution of the phonon softening associated with the Kohn anomaly. We then connect these strain trends to electron-phonon quantities relevant for Eliashberg theory, in particular the spectral function $\alpha^2F(\omega)$, the coupling constant λ, and characteristic phonon frequencies. By combining these ingredients, we compute the superconducting critical temperature T_c as a function of applied strain.

Overall, this work provides a microscopic perspective on strain engineering in conventional superconductors and is intended to offer concrete theoretical guidance for future experimental studies exploring strained Nb systems.

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P35

Polaron-Driven Transport and Exciton–Phonon Coupling in Nitride Perovskites: A First-Principles Perspective

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Abstract

Nitride perovskites are emerging as a class of polar semiconductors characterized by strong lattice polarization, stable vibrational spectra, and moderate electronic band gaps. Using density-functional theory and density-functional perturbation theory, we investigate their structural, electronic, vibrational, optical, and thermoelectric properties. We find that these materials exhibit stable polar optical phonons, large lattice contributions to the dielectric response, elastic anisotropy, and strong optical absorption, together with unusually large Seebeck coefficients.These ground-state and linear-response properties provide direct evidence that charge carriers and optical excitations in nitride perovskites are strongly influenced by lattice vibrations. The coexistence of polar phonons, dielectric screening, and dispersive electronic bands places these materials in a regime where electron–phonon coupling, polaron formation, and phonon-assisted optical processes are expected to play a dominant role in transport and optical response. The present results therefore establish a robust first-principles foundation for advanced many-body treatments of nitride perovskites. They motivate future calculations based on EPW, GW, and Bethe–Salpeter approaches to quantify electron–phonon coupling strengths, quasiparticle renormalization, and exciton–phonon effects from first principles.

Keywords - Electron–phonon coupling; Polaronic transport; Exciton–phonon interactions; Nitride perovskites; Density-functional perturbation theory (DFPT); First-principles calculations;

P36

Spatially Resolved Photoluminescence of Interlayer Excitons in Transition Metal Dichalcogenide Heterostructures

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Transition metal dichalcogenides (TMDs) are atomically thin semiconductors that host extraordinarily strong Coulomb and light-matter interaction. The optical response of TMD heterostructures is dominated by interlayer excitons (IXs), exhibiting large binding energies on the order of hundreds of meV and long photoluminescence lifetimes.
In addition to the optically accessible bright excitons, there also exists a multitude of optically forbidden dark excitons. Bright and dark states are coupled via exciton-phonon scattering, which leads to phonon-induced sidebands and an asymmetric excitonic line shape [1].
Recent experiments using spatially ring-shaped optical excitations of IX ensembles reveal the accumulation of excitons in the rings' center. Accompanied by asymmetric spectral lineshapes, this suggests a spatial propagation of high-energy IXs [2]. Within this contribution, we present a microscopic theory for the spatially resolved photoluminescence of inhomogeneous IX ensembles. By explicitly incorporating both the relative and center-of-mass momentum in the Wigner function, we investigate the impact of spatial exciton propagation and exciton-phonon scattering on the asymmetric emission lineshape.

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P37

Pressure-Driven Enhancement of Conventional Superconductivity in Symmetry Reduced Multicomponent Hydride-Derived systems

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Abstract

We investigate conventional superconductivity in a class of multicomponent hydride-derived systems obtained through systematic compositional substitution and symmetry lowering from a high-symmetry parent lattice. Using first-principles density functional theory combined with density functional perturbation theory, we perform a comparative study of the electronic structure, lattice dynamics, and electron–phonon coupling under hydrostatic pressure. Reduction of the crystallographic space-group symmetry leads to band folding and enhanced orbital hybridization near the Fermi level, resulting in pressure-tunable van Hove singularities in the electronic density of states. These singular features are found to amplify the electron–phonon coupling constant through selective softening of high-frequency hydrogen-dominated phonon modes.

We demonstrate that pressure not only stabilizes the dynamically favorable low-symmetry phases but also drives a non-monotonic evolution of the superconducting critical temperature, governed by the interplay between Fermi-surface topology, phonon linewidth enhancement, and anharmonic effects. Comparative analysis across structurally related systems reveals that symmetry reduction acts as a key control parameter for engineering enhanced superconducting responses without invoking strong electronic correlations. Our results establish a general design principle for pressure-induced superconductivity in complex hydride frameworks, highlighting the role of van Hove singularity engineering within an electron–phonon-mediated pairing paradigm.

P38

First-principles quasi-harmonic study of phase competition in $NaNbO_3$

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Sodium niobate ($NaNbO_3$) is known among the perovskite oxides for its complex and poorly-resolved progression of structural phases with temperature [1]. While related oxide perovskite chemistries such as potassium niobate and calcium titanate exhibit structural phase behavior which is amenable to crystal-chemical heuristics based on ionic coordination, $NaNbO_3$ is ill-suited to interpretation with these simple models. Here, we present a study of the energetics and thermodynamics of the known low- and room-temperature structrual phases of $NaNbO_3$ using first-principles calculations and a quasi-harmonic construction of the vibrational free energy of these phases between 0-500 K, in an attempt to resolve open questions on the stability and phase selection of the experimentally observed room-temperature antiferroelectric (AFE) P-phase with space group $Pbcm$. Our findings suggest that such vibrational contributions to the free energy may be important in favoring the AFE P phase over its ferroelectric counterpart Q. Furthermore, the slight instability of a Γ-point phonon mode at around $30i$ cm^{-1}, which is known to appear in first-principles studies of the P phase [2], is potentially suppressed by zero-point energy contributions, bringing into question the feasibility of the proposed $Pca2_1$ structure for $NaNbO_3$.

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P39

Non-perturbative theory of the electron-phonon coupling and its first-principles implementation

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The contribution of nuclear dynamics and electron-phonon interactions to material properties is commonly evaluated using the harmonic approximation for ionic fluctuations and a linear coupling framework between phonons and electrons. However, this approach may not hold when quantum and anharmonic effects play a dominant role—such as in hydrogen-based systems, high-T_c superconductors, or materials near charge-density wave or ferroelectric phase transitions. In these cases, the validity of traditional methods becomes questionable. In this contribution, we present a non-perturbative method that includes nonlinear effects and accounts for the quantum nature of nuclei. The approach is based on the $GW^{(en)}$ approximation for the electron self-energy, incorporating the effective nuclei-mediated electron-electron interaction ($W^{(en)}$) and the electron Green's function (G). Nuclear dynamics are described using a Gaussian distribution function, which captures anharmonicity at the mean-field level. The Debye-Waller-renormalized average vertices, computed stochastically in supercells, are central to this method. A first-principles implementation of the approach is presented, compatible with the stochastic self-consistent harmonic approximation. Validation of the method in aluminum—a highly harmonic system— yields results that are consistent with standard linear electron-phonon calculations. In contrast, calculations for palladium hydride, which is strongly anharmonic, reveal substantial nonlinear corrections to the electron-phonon interaction. This method holds significant potential for improving *ab initio* calculations of properties related to electron-phonon interactions, such as superconductivity and electrical conductivity, in anharmonic systems.

P40

Unveiling a Phonon-Mediated Pathway for Structural Transformation in Yttrium

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Understanding the mechanism of structural phase transitions in rare-earth elements is a fundamental challenge in condensed matter physics, with significant implications for materials science applications. In this study, we present a systematic investigation on the phase transitions of yttrium under pressure conditions (<30 GPa) focusing on the *hcp*, *Sm-type*, and *dhcp* phases. A comparative study between the GGA and meta-GGA functionals reveals that the PBE functional significantly underestimates the phase transition pressures, whereas the r^{2}SCAN functional provides accurate predictions of phase transition pressures which are in excellent agreement with experimental data [1]. The solid-state nudge elastic band calculations reveal a low activation barrier for the hcp to Sm-type phase transformation, transformation hcp to host-guest phase transition, in contrast to the behaviour observed in scandium [2]. Phonon dispersion calculations uncover pronounced softening of acoustic modes in both the hcp and Sm-type phases as pressure increases. These soft modes, accompanied by pressure-induced *s* to *d* charge transfer, signalling a strong coupling between electronic redistribution and lattice vibrations. A detailed analysis of the soft-mode further reveals a new intermediate phase of P$\bar{6}$2c symmetry occurring during the transition between the hcp and Sm-type phase. A transition from the centrosymmetric space group P6$_3$/mmc (hcp) to the t-type subgroup P$\bar{6}$2c involves loss of inversion symmetry and a reduction in point group symmetry from D$_{6h}$ to D$_{3h}$. Additionally, calculations of elastic properties confirm mechanical softening at the phase boundaries, particularly in the hcp phase, suggesting a strong correlation between elastic softening and structural transitions. These findings indicate that the emergence of soft modes in the phonon dispersion curves along is a key factor driving structural phase transition in the rare-earth materials.

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P41

Phonon self-energy correction in phonon-mediated nonlinear optical conductivity

P42

Negative mobility and electron hole bifluidity in doped graphene

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In this poster, I discuss the curious phenomenon of negative differential conductivity and hydrodynamic transport of charge carriers in doped graphene, connected to some recent measurements [1]. To probe this physics, we extend the *ab initio* `elphbolt` [2] transport code to include the Coulomb collision integral. We find that the strong Coulomb interactions can not only drive the individual hydrodynamics in the electron and hole subsystems, but also the far more exotic joint electron-hole bifluidity [3]. Furthermore, we observe a strong violation of the Wiedemann-Franz law closer to the charge neutrality condition. These findings establish the roles of microscopic scattering mechanisms for achieving the hydrodynamic transport state in electron-hole systems. I also discuss the computational challenges and our ongoing efforts in extending this work.

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P43

Phonon-assisted light absorption and emission in cubic boron nitride

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(Dated: 25 March 2026)

Cubic boron nitride (cBN) is a wide-bandgap semiconductor whose optical properties remain poorly understood. Experiments report optical features in the 6–7 eV range, whereas first-principles many-body calculations predict a much larger direct optical gap, close to 11 eV. This long-standing discrepancy suggests that indirect, phonon-assisted processes play a central role in the optical response of cBN.[1–4]

In this work, we investigate the absorption and luminescence of cBN from first principles. Our approach combines GW quasiparticle corrections, the Bethe–Salpeter equation, and exciton–phonon coupling within a unified many-body framework. This allows us to describe excitonic effects and phonon-assisted optical transitions on the same footing, and to assess whether indirect excitonic processes can explain the low-energy optical features observed experimentally.[4,5]

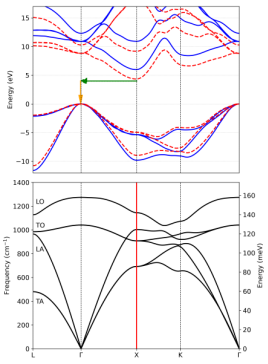

FIG. 1. Top: electronic band structure calculated at the Kohn–Sham (red dashed line) and G_0W_0 (blue solid line) levels. The lowest phonon-assisted transitions are indicated by the green and orange arrows. Bottom: phonon band structure. The phonons at $\mathbf{q} = X$ responsible for the lowest phonon-assisted valence-to-conduction transitions are highlighted.

We find that phonon-assisted transitions make a strong, and in practice dominant, contribution to both absorption and emission. When exciton–phonon coupling is included, the calculated spectra shift substantial spectral weight to lower energies and move significantly closer to experiment. These results show that the optical response of cBN cannot be interpreted from the direct gap alone. Atomic vibrations must be treated explicitly, since they open indirect optical channels and strongly reshape the excitonic spectrum.

More broadly, our results place cBN within the wider boron nitride family, where strong exciton–phonon coupling is already known to produce efficient light emission even in indirect-gap systems. cBN therefore provides another important example in which phonons are not a small correction, but a key part of the luminescence mechanism. Our work helps reconcile theory with experiment and provides a clearer picture of light emission in wide-bandgap boron nitride materials.[6,7]

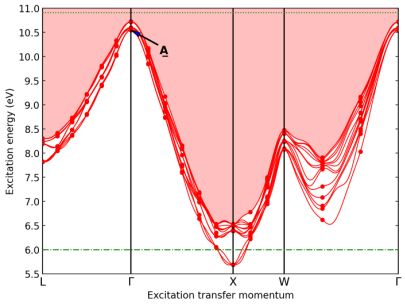

FIG. 2. Excitonic dispersion of cBN. The label A marks the bright exciton peak close to the lowest bundle of states at Γ.

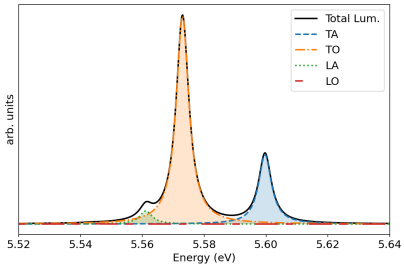

FIG. 3. Total phonon-assisted luminescence of cBN (solid line) and the contributions from the different phonon modes at $q = X$: LO branch (red dashed line), LA branch (green dotted line), TO branch (orange dash-dotted line), and TA branch (blue dashed line).

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P44

Intertwined charge density wave instability and superconductivity from electron-phonon coupling

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The emergence of charge density wave (CDW) order and superconductivity in low-dimensional materials remains an important topic in condensed matter physics [1, 2, 3]. Using first-principles calculations, we have investigated lattice instability and superconductivity in a janus transition metal dichalcogenide (TMDC) monolayer derived from a known CDW system. The calculated phonon dispersion displays a clear softening of an acoustic branch at the M point of the irreducible Brillouin zone, indicating the emergence of a CDW instability. A comprehensive investigation regarding the electron-phonon coupling strength and the real part of static Lindhard charge susceptibility has been carried out. Our findings indicate that this anomaly is linked to the enhanced electron-phonon interaction and electronic instability arising from both interband and intraband scattering. The corresponding structural distortion reconstructs the band structure, lowers the crystal symmetry by breaking both rotational and mirror symmetries, and opens a small indirect band gap, driving the system from a semimetallic to a semiconducting state. The effect of electronic correlation is further investigated, demonstrating that it offers an effective route to tune the robustness of the CDW distortion. Within the Migdal-Eliashberg formalism implemented in Electron Phonon Wannier (EPW) code [4, 5, 6], we have further investigated superconductivity in the undistorted high temperature phase. In the undistorted phase, the system exhibits phonon mediated anisotropic two-gap superconductivity originating primarily from robust coupling between electronic bands crossing the Fermi level and the soft phonon mode at the M point. Our results highlight the key role of electron-phonon interaction in governing the emergence of both CDW order and superconductivity in low-dimensional materials.

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P45

Coupled electron-phonon hydrodynamics and Viscous Thermoelectric Equations

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Non-diffusive, fluid-like transport of charge and heat has been observed in several materials, raising the question of whether they can emerge simultaneously and how they are related to electron-phonon two-component fluids. We introduce a first-principles theory and computational framework to quantitatively describe these phenomena from atomistic to continuum scales in complex device geometries. Starting from the microscopic coupled electron-phonon Boltzmann transport equation, we formalize the emergence of composite "relaxon" electron-phonon excitations, show that they determine the viscosity tensors of the two fluids, and quantify the impact of electron-phonon drag on thermoelectric transport coefficients. We then demonstrate that the coupled Boltzmann equation can be coarse-grained into a set of mesoscopic Viscous Thermoelectric Equations, formally unifying Gurzhi's hydrodynamic equation for electrons [1] and the recently developed Viscous Heat Equations for phonons [2], while extending them to cover the intermediate regime of mixed electron and phonon fluids. We leverage this framework to elucidate how electron and phonon fluids can coexist or mix, rationalizing pioneering experiments on electron-phonon drag in graphite, and predicting smoking-gun signatures of nondiffusive behavior such as nonharmonic temperature and electric potential fields, and compressible thermoelectric backflow.
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P46

Strain-Driven Control of Hall Transport and Optical Absorption in Monolayer AsTeBr

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Two-dimensional materials hosting nontrivial Berry curvature have emerged as a promising platform for realizing unconventional Hall responses beyond the linear regime [1–3]. In this work, we investigate the strain-tunable topological and optoelectronic properties of monolayer AsTeBr using first-principles density functional theory calculations including spin–orbit coupling. The broken inversion symmetry in AsTeBr gives rise to a pronounced Berry curvature near the band extrema, leading to a sizable nonlinear anomalous Hall conductivity even in the absence of an external magnetic field. Biaxial strain is applied over a wide range from 0% to $+6\%$ to explore the interplay between lattice deformation, electronic structure, and topological response. We find that tensile strain induces an indirect-to-direct band gap transition at $+6\%$, which persists under further tensile strain. This transition significantly enhances optical transition probabilities. Simultaneously, strain strongly modulates the Berry curvature distribution in momentum space, resulting in a tunable nonlinear anomalous Hall response. In particular, tensile strain enhances the Berry curvature dipole, leading to an increased magnitude of the nonlinear anomalous Hall conductivity [4]. In addition, we analyze the strain-dependent optical properties by calculating the frequency-dependent dielectric function and optical absorption spectrum. The emergence of a direct band gap under tensile strain leads to a redshift of the absorption edge and enhanced absorption in the visible range, highlighting the potential of strained AsTeBr for optoelectronic applications. Our results establish monolayer AsTeBr as a versatile strain-engineered quantum material in which topology, nonlinear transport, and optical response can be simultaneously controlled, offering a viable platform for next-generation Hall-based and optoelectronic devices.

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P47

Electron-phonon Renormalization in Momentum-resolved Electronic Structure of Scandium Nitride

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Electron-phonon interactions play a crucial role in renormalizing quasiparticle energies and governing transport properties in solids [1,2]. Yet, their momentum-resolved impact on electronic band structures and lifetime broadening remains largely unexplored. Here, we present a combined high-resolution angle-resolved photoemission spectroscopy (ARPES) and first-principles density functional theory (DFT) calculations to investigate phonon-induced renormalization of electronic band structure in semiconducting scandium nitride (ScN). Both ARPES and DFT calculations reveal clear deviations from a single-particle band picture, including a pronounced photoemission kink ~2.3 eV below the valence-band maximum and substantial broadening of states across the Brillouin zone. To interpret these features, we employ Wannier function perturbation theory [3] within the non-adiabatic Allen-Heine-Cardona formalism [4] to compute the electron-phonon self-energies and quasiparticle spectral functions. The calculations reproduce the observed dispersion anomalies and lifetime broadening, identifying electron-phonon coupling as the dominant mechanism. Additionally, the experimentally observed unusual temperature-dependent increase in the direct band gap is accurately captured by incorporating both thermal expansion and electron-phonon renormalization. These findings identify ScN as a model semiconductor, providing a well-defined platform for understanding the role of electron-phonon coupling in the renormalization of the electronic-structure of nitride materials.

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P48

Electron–Phonon Coupling in the Double Perovskite La_2MnNiO_6: A First-Principles FP-LAPW Study as a Starting Point for Many-Body Treatments

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Double perovskite oxides based on transition metals provide a fertile platform for investigating the interplay between lattice, charge, spin, and orbital degrees of freedom. In this work, we present a first-principles study of the double perovskite La_2MnNiO_6 using Density Functional Theory (DFT) within the full-potential linearized augmented plane-wave (FP-LAPW) method as implemented in the ELK code [1].

We establish a reliable electronic ground state by analyzing crystal-field effects, spin polarization, and orbital-resolved electronic structure, with particular emphasis on Mn–Ni–O hybridization and its impact on low-energy electronic excitations. Based on the symmetry and character of the electronic states near the Fermi level, we discuss the coupling between lattice vibrations and electronic degrees of freedom, identifying phonon modes expected to play a dominant role in electron–phonon interactions [2, 3].

Although the present results are obtained at the DFT level, they are explicitly designed to serve as a benchmark and starting point for many-body perturbation theory approaches. In particular, we outline how the FP-LAPW electronic structure can be interfaced with density functional perturbation theory for phonons, Migdal–Eliashberg theory for electron–phonon coupling, and GW-based quasiparticle corrections. Expected many-body effects such as phonon-induced band renormalization and correlation-enhanced coupling strengths are briefly discussed.

Our results position La_2MnNiO_6 as a promising material platform for systematically bridging accurate all-electron DFT calculations with many-body descriptions of electron–phonon physics in correlated oxide systems.

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P49

Concerted rattling-induced strong anharmonicity and phonon coherence lead to ultralow glasslike thermal conductivity in TlAgTe

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Ordered crystalline materials exhibiting ultralow and glasslike thermal conductivity are of significant fundamental and technological interest, particularly for thermal management and thermoelectric applications. In such systems, heat transport is dominated by phonon quasiparticles, yet the microscopic mechanism underlying glasslike transport in ordered crystals remain elusive.

In this poster, I will show state-of-art first-principles calculations based on density functional theory to investigate the experimentally observed ultralow thermal conductivity in TlAgTe. This compound features disconnected Tl atomic chains embedded with a three-dimensional framework of distorted $AgTe_4$ tetrahedra. Using a unified anharmonic lattice dynamics framework that incorporates phonon self-energy frequency renormalization [1], three- and four-phonon [2,3] scattering process and both particlelike (κ_l^P) and wavelike coherent (κ_l^C) transport contributions, we calculate the lattice thermal conductivity that agrees very well with the experiments in both magnitude and temperature dependence. Our analysis reveals multiple localized phonon modes arising from concerted rattlinglike vibrations of Tl and Ag atoms. These modes exhibit strong temperature dependence and enhanced four-phonon Umklapp scattering, drastically supressing the particlelike contribution (κ_l). Additionally, strong anharmonicity driven by local structural distortions and lone-pair electrons induces a crossover from particlelike to wavelike (coherent tunnelling) phonon transport above ~40 cm^{-1}, leading to a significant κ_l^C contribution.

Therefore, we show direct structure-property relationship linking local rattling, strong anharmonicity, and phonon coherence. These principles can be used for materials design with tuneable ultralow thermal conductivity.

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P50

Coupling Molecular Dynamics Simulation to the Multiple Scattering Calculations : Application to the Time Resolved X-Ray Photoelectron Diffraction (TR-XPD)

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In modern times, our reliance on electronic devices is steadily increasing. These devices are built from materials whose performance is often determined by their atomic structure. And sometimes even the smallest structural variation can alter the performance. Thus, we need to measure such structural details accurately. X-ray photoelectron diffraction (XPD) is a powerful experimental technique for this purpose. It offers several key advantages, including high surface sensitivity, chemical specificity, and the ability to resolve the local geometric environment of atoms with remarkable precision. With recent technological advancement, experiments can now achieve time resolutions of the order of femtoseconds, enabling researchers to observe the ultrafast dynamics of chemical reactions at the material surfaces. This level of insight provides invaluable tools for uncovering material properties not only at the atomic levels but also at the reaction time scale. However, such time resolved XPD experiments are extremely complex and rarely available, often making it difficult to directly extract complete structural information from raw measurements alone.

To overcome this challenge, it becomes essential to model the experimental system. Our work addresses this problem by integrating material modelling approach to investigate the real-time structural evolution of materials. This focuses on developing a computational modeling framework that quantitatively connects atomic motion obtained from molecular dynamics (MD) simulations with measurable spectroscopic observables through multiple scattering (MS) theory. This allows us to gain a deeper, more comprehensive understanding of the time-resolved X-ray photoelectron diffraction(TR-XPD) for materials surface analysis.

P51

Real-Space formalism for phonons within density functional perturbation theory

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Abstract:

We present a real-space formulation of density functional perturbation theory for the calculation of phonons. Specifically, employing a local exchange-correlation functional, norm-conserving pseudopotential in the Kleinman-Bylander representation, and local form for the electrostatics, we derive expressions for the dynamical matrix and associated Sternheimer equation that are particularly amenable to the real-space finite-difference method. In particular, the formulation is applicable to insulating as well as metallic systems of any dimensionality, enabling the efficient and accurate treatment of semi-infinite and bulk systems alike, for affine as well as non-affine geometries. Through representative examples, we demonstrate the accuracy and efficiency of the developed formulation and implementation.

P52

First-principles many-body study for electronic, optical, and excitonic properties of RbTlCl3 perovskite for solar cells

P53

Spin-Split Phonon-Limited Carrier Mobilities from Electron-Phonon Coupling in 2D VX_2 (X = S, Se) Bipolar Magnetic Semiconductors

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The study investigates phonon-mediated charge carrier mobility in ferromagnetic 2D vanadium-based transition metal dichalcogenides (TMDCs), specifically VX_2 monolayers (X = S, Se) as intrinsic bipolar magnetic semiconductors (BMS). These materials feature a distinctive electronic structure with the semiconducting gap between spin-up and spin-down bands, valence band maximum dominated by spin up channel and conduction band minimum by the opposite spin down yielding pronounced spin-split band edges from intrinsic magnetic moments. This enables intrinsic spin filtering and gate-tunable spin polarization without external fields, making them highly promising for advanced spintronics such as bipolar spin-filtering transistors, low-power magnetic random-access memory (MRAM), and non-volatile spin logic devices. Carrier transport in these magnetic 2D materials is crucial for fundamental understanding and applications in storage and spintronics, as phonon-limited mobility defines the upper limits of charge transport efficiency and switching speeds under electron-phonon coupling. Using the Electron-Phonon Wannier (EPW) code within the Quantum ESPRESSO framework, we performed first-principles calculations of phonon-limited electron and hole mobilities, with the local spin density approximation (LSDA) to capture ferromagnetic ordering and spin-dependent effects. Hole mobility is primarily dominated by acoustic phonons, while electron mobility is mostly limited by optical phonons. A pivotal result is the significant mobility enhancement upon applying GW quasiparticle corrections, which correct self-interaction errors in DFT, reduce effective masses, and improve band curvature. In this, the hole mobility suppressed intervalley scattering due to dominant effective mass reduction in case of VS_2 and the absence of intervalley scattering further promotes high hole mobility in VSe_2. This work elucidates intrinsic transport limits in 2D VX_2, highlights the role of electron-phonon interactions in spin-split systems, and supports the design of ultra-low-power, robust spintronic devices based on vanadium dichalcogenides, advancing the field of 2D magnetic semiconductors for next-generation nanoelectronics.

P54

Strain induced tunable band gap and optical properties of graphene on hexagonal boron nitride

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In this study[1], we highlight the potential of strain engineering in graphene/hexagonal boron nitride (hBN) 2D heterostructures, enabling their use as wide-range light absorbers with significant implications for optoelectronic applications. We systematically investigate the electronic and optical properties of graphene/hBN under the application of strain, considering various stacking geometries within the framework of density-functional theory. The semimetallic graphene layer upon aligning on the insulating hBN sheet opens a few tens of meV band gap at the Dirac point caused by the breaking of sublattice symmetry through induced on-site energy variations. Here, we demonstrate that by simultaneously tuning the interlayer distance and lattice constant, this band gap can be significantly increased to 1 eV. Interestingly, in both scenarios (small and large band gaps), the material undergoes a transition from a semiconductor to a narrow gap state. Importantly, the tunability of this band gap is strongly influenced by the specific stacking configuration. We further explored the optical properties across a broad spectrum, revealing that the presence of a strain-induced band gap fundamentally alters how light interacts with the system.

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P55

Phonon-induced superconductivity in rhombohedral multilayer graphene from first principles

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Following the discovery of superconductivity in twisted moiré graphene heterostructures, superconductivity has been observed, too, in untwisted rhombohedrally stacked multilayer graphene [1,2], triggering significant interest in the mechanisms driving superconductivity in these systems. Although the microscopic origin remains under active debate, earlier studies based on phonon-mediated pairing have shown that electron–phonon coupling can account for both the observed superconducting transition temperatures and the emergence of chiral superconducting states in multilayer graphene [3,4]. However, some of the approximations employed in these works may break down in this unconventional superconducting environment. In this work, we apply multiband Migdal–Eliashberg theory [5], combined with *ab initio* inputs, to compute the superconducting properties of rhombohedrally stacked multilayer graphene. From first-principles calculations, we find that phonon modes associated with interlayer coupling are the most likely candidates for superconducting pairing. We find that, despite open questions that call for further experimental and theoretical investigation, the principal experimental observations can be consistently explained within an electron–phonon–mediated framework.

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P56

A New Approach to Variable-Cell Structural Relaxation of Anharmonic Crystals in Finite-Temperature and High-Pressure Conditions

Accurately determining crystal structures under finite temperature and pressure remains one of the central challenges in computational solid-state physics. Standard methods such as the quasi-harmonic approximation (QHA) often lose reliability in systems dominated by strong anharmonic effects—hydrides and other light-element compounds being prime examples. Molecular dynamics (MD) simulations naturally incorporate full P, T dependencies, but their computational cost grows rapidly with system size and simulation length, and they typically provide access only to time-averaged structural information.

The Temperature-Dependent Effective Potential (TDEP) method offers an appealing alternative by capturing anharmonic behavior through force-constant fitting to thermally sampled configurations. This approach enables the construction of temperature-dependent phonon spectra and free energies while remaining significantly more efficient than MD.

In this work, I will present a new extension of the TDEP framework designed specifically for performing finite-temperature structural relaxations at high pressure. The method provides a direct route to equilibrium crystal geometries in regimes where anharmonicity is essential and traditional tools fail, thereby improving predictive accuracy for materials under extreme conditions.

P57

Local structural distortions, hydrogen bonding, and vacancy defects in hybrid perovskites from first-principles

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First-principles calculations provide key insights into the structural and electronic properties of hybrid lead halide perovskites, particularly in systems with compositional complexity and intrinsic defects. In mixed-cation $FA_xMA_{1-x}PbI_3$ perovskites[1] our calculations reveal that cation substitution at the *A* site induces significant tilting of the PbI_6 octahedra, which plays a dominant role over the unit-cell volume in determining the band gap. The calculations further show that hydrogen bonding between organic cations and iodine anions is preserved across the entire compositional range, with MA–I interactions remaining consistently stronger than FA–I ones. These interactions stabilize the non-bonding I-*5p* orbitals, lowering their energy and contributing to the structural stability of the material. On the other hand, performing ab initio two-component DFT calculations one can obtain positron lifetimes that allow to identify the chemical nature of intrinsic defects. Our calculations for $CH_3NH_3PbBr_3$[2], one of the most promising materials for tandem solar cells, demonstrate that the positron lifetime associated with lead vacancies is highly sensitive to the local environment of the vacancy and not necessarily on the disorder of the structure used to describe the perovskite crystal. Our results agree with the value measured in single crystals and importantly suggest that the growth conditions strongly influence the chemical nature and the concentration of the defects present in the bulk of this material.

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P58

Dragful magnetotransport in `elphbolt`

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The incorporation of magnetic field effects into charge and heat transport is essential for modeling a wide range of solid-state phenomena, from magnetoresistive sensors to thermomagnetic energy conversion. When a magnetic field is present, transport coefficients depend on the field strength and orientation, giving rise to galvanomagnetic and thermomagnetic effects such as the Hall, Nernst, Ettinghausen, and Righi–Leduc effects [1]. At present, however, there is no computational tool that can compute magnetotransport while taking into account the electron-phonon drag effect in a fully self-consistent manner. This work fills this gap by introducing a complete theory and corresponding implementation in the `elphbolt` [2] computational package for the coupled electron–phonon Boltzmann transport equations in the presence of a magnetic field, with strictly enforced Onsager reciprocal relations [1].

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P59

Probing Electron-Phonon Interaction with Resonant Inelastic X-ray Scattering

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Resonant inelastic X-ray scattering (RIXS) is a photon-in/photon-out spectroscopic technique that accesses elementary excitations involving various degrees of freedom (spin, charge, lattice, etc.)[1, 2]. Recent progress in synchrotron facilities has made it possible to access phonon excitations with remarkably high resolution, providing momentum dependence, element selectivity, and bulk sensitivity. However, interpreting RIXS spectra remains challenging due to the coupling between different excitations. Indeed, although RIXS is used to measure electron–phonon coupling [3], it primarily reveals exciton-phonon coupling, due to the interaction with a core hole [4]. So far, theoretical approaches mainly rely on oversimplified models that use adjustable parameters to fit experimental results, limiting their applicability [5].

The Bethe–Salpeter equation (BSE) represents the state-of-the-art method for describing excitonic effects, as it explicitly accounts for electron–hole correlation, and has been successfully applied to reproduce X-ray absorption and RIXS spectra [6, 7]. Building on this approach, we propose an ab initio method to compute phonon excitations in RIXS by combining the BSE with Density Functional Perturbation Theory (DFPT). In this work, we will discuss the role of exciton–phonon interactions in RIXS spectra and present preliminary results for hexagonal boron nitride (hBN).

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P60

Electron phonon coupling in presence of strong correlations: possible low-energy models

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The microscopic origin of high temperature superconductivity in cuprates remains one of most debated questions in condensed matter physics. The presence of strong electron correlations makes these systems challenging. Recent advances in experimental techniques reveal a complex interplay of quasiparticles such as electrons, phonons, and magnons [1].

With the aim of understanding the interplay between these quasiparticles, we plan to undertake a theoretical study of the cuprate $Ca_2CuO_2Cl_2$ (CCOC) [2] by following a multi-tier approach. Starting from a density functional theory description of the electronic structure, we include phonon effects as computed by the density functional perturbation theory. Finally strong electronic correlation is modelled by a local Hubbard repulsion, resulting in a model that can be tackled with extended dynamical mean field theory [3]. We present the overall plan by discussing possible ways of deriving model Hamiltonians within this framework.

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P61

Phonon screening of excitons in the Ruddlesden-Popper structure of $SrTiO_3$

P62

Valley differences in monolayer MoS_2 calculated with the GW approximation

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Transition metal dichalcogenides (TMDs) are leading candidates to succeed silicon in next-generation transistors. Their atomic thickness and lack of dangling bonds enable extreme device scaling. However, realizing this potential requires a deep understanding of their electronic properties, which are fundamentally governed by complex scattering mechanisms and many-body effects.

The band structure of monolayer TMDs features distinct valleys in the conduction and valence bands. While the direct band gap occurs at the K point, an additional conduction band valley at the Q point (located between Γ and K) becomes accessible at high electron densities. The occupation of these multiple valleys significantly enhances electron-phonon scattering [1], making the relative energy offset between the K and Q valleys a critical parameter for device performance.

In this work, we investigate these valley differences in monolayer MoS_2 using the GW approximation. By comparing our in-house quantum transport code with G0W0 calculations, we demonstrate that GW corrections reduce the conduction band valley offset compared to standard Density Functional Theory (DFT) predictions. Finally, we incorporate these GW renormalized energies and electron-electron scattering effects into quantum transport simulations to evaluate their impact on the electrical current.

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