CMT@BRIXEN

26th-28th August 2026

The Meeting of the Condensed Matter Theory Italian Community

PROGRAM & BOOK OF ABSTRACTS

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Emergent topological states in semiconductor-ferromagnet van der Waals heterostructures

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Program

Tuesday the 25th of August 2026

Welcome Dinner (20:00 – Il Grissino)

Wednesday the 26th of August 2026

From 8.00 onwards Registration

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Advances in First Principles Simulations (9:00-12:30) – Chair: Marco Gibertini

9:00-9:50 Keynote: **Nicola Marzari (EPFL, PSI and Cambridge University) – *Excitations and Correlations from Functional Theories***

9:50-10:20 Invited: **Fulvio Paleari (CNR-NANO) – *Efficient Calculation of Exciton-Phonon Matrix Elements for Spectroscopy and Nonequilibrium Dynamics***

Coffee Break (10:20-11:00)

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11:20-11:40 Contributed: **Paolo Fachin (University of Rome La Sapienza) – *Galilean invariant non-adiabatic vibrational dynamics in pseudo-potential and tight-binding methods***

11:40-12:00 Contributed: **Nina Girotto Erhardt (University of Louvain) – *Self-Consistency in Electron Spectral Functions and Transport***

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Spectroscopy and Ultrafast Phenomena (14:30-18:00) – Chair: Matteo Calandra Buonaura

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17:10-17:30 Contributed: **Andrea Biondini (University of Modena and Reggio Emilia) – *Molecular Nitrogen in Wide-Bandgap Nitrides: Connecting RIXS and Photoluminescence from First Principles***

17:30-18:00 Invited: **Stefano Mocatti (University of Trento) – *A Unified First-Principles Approach to Photocarrier and Phonon Dynamics in Photoexcited Materials***

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Materials for Energy (9:00-12:50) – Chair: Alice Ruini

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11:00-11:20 Contributed: **Francesca Martini (University of Trento) – *High-Throughput First-Principles Screening of Surface Work Functions for Water Splitting Applications***

11:20-11:40 Contributed: **Andrea Droghetti (Ca' Foscari University of Venice) – *Electronic Correlations in Nanodevices under Bias***

11:40-12:00 Contributed: **Michele Bagaglini (University of L'Aquila) – *Twistronic Control of Shift Current in Multilayer Moiré System***

12:00-12:30 Invited: **Paolo Pegolo (EPFL) – *Coupled Heat and Charge Transport from Equilibrium Molecular Dynamics***

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Machine Learning in Condensed Matter Physics (14:00-17:30) – Chair: Silvana Botti

14:00-14:50 Keynote: **Paul Erhart (Chalmers University of Technology) – *Accelerating Advanced Simulations by Machine Learning: From Models to Insight***

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15:20-15:40 Contributed**: Sita Schoenbauer (Technical University of Vienna) – *Machine-Learned Force Fields for Lattice Dynamics at Coupled-Cluster Level Accuracy***

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16:40-17:00 Contributed **Daniela Mangano (University of Bologna) – *Nonadiabatic polaron dynamics from machine-learned hopping trajectories***

17:00-17:30 Invited: **Andrea Grisafi (University of Sorbonne) – *Machine Learning of Electronic Charge Densities in the Simulation of Electrochemical Interfaces***

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Friday the 28th of August 2026

Session Magnetism, superconductivity and topology (9:00-12:30) – Chair: Gianni Profeta

9:00-9:50 Keynote: **Maia Vergnory (University of Shebrooke and DIPC) – *From Theory to Materials: The Search for Topological Quantum Matter***

9:50-10:20 Invited: **Dario Fiore Mosca (University of Vienna) – *Effect of Doping on Double Perovskites: From Polarons to Hidden Orders***

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11:00-11:20 Contributed: **Luigi Camerano (University of L'Aquila) – *Multiferroic Altermagnetism and Magneto-Orbital Excitations in Monolayer VCL***

11:20-11:40 Contributed: **Johanna Paulina Carbone (University of Vienna) – *Polaron-mediated anisotropic exchange in two-dimensional magnets***

11:40-12:00 Contributed: **Srdjan Stavric (Vinča Institute of Nuclear Sciences) – *Emergent nonreciprocity in a p-wave magnet NiI2: Descriptors for data-driven functional materials***

12:00-12:30 Invited: **Zeila Zanolli (Utrecht University) – *Density Functional Bogoliubov-De Gennes Theory for Superconductors***

Concluding Remarks (12:30-12:50)

ABSTRACTS OF TALKS

Wednesday the 26th of August 2026

Advances in First Principles Simulations (9:00-12:30)

9:00-9:50 Keynote: Nicola Marzari

EXCITATIONS AND CORRELATIONS FROM FUNCTIONAL THEORIES

Nicola Marzari

Theory and Simulation of Materials, EPFL and PSI
Theory of Condensed Matter, Cavendish Laboratory, University of Cambridge

Density-functional theory has shaped our understanding of materials, and even its shortcomings offer opportunities for deeper insight. I will trace our practical and conceptual progress, beginning with a brief recall and reinterpretation of Hubbard functionals, which enable an efficient and more accurate treatment of the chemistry of localised electrons by enforcing a heuristic condition of piecewise linearity. Generalising this condition to all orbitals leads to Koopmans functionals, marking a conceptual advance: functionals of the orbital densities can predict spectral properties (from charged excitations to band gaps) while unencumbered from the acrobatics of derivative discontinuities. I will then introduce a broader framework: a functional theory of the occupied spectral density, and its application to paradigmatic correlated solids. This approach captures both excitations and electronic correlations within a functional formulation, leading to new theorems, algorithms, and capabilities in an expanded domain.

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[1] *Energies and spectra of solids from the algorithmic inversion of dynamical Hubbard functionals* (T. Chiarotti, A. Ferretti, T. Marzari)
[2] *Functional theory of the occupied spectral density* (A. Ferretti, N. Marzari)
[3] *Dynamical Hubbard approach to correlated materials: the case of transition-metal monoxides* (M. Caserta, T. Chiarotti, M. Vanzini, N. Marzari)
[4] *Self-consistent dynamical Hubbard functional for correlated solids* (T. Chiarotti, M. Quinzi, A. Pintus, M. Caserta, A. Ferretti, N. Marzari)

9:50-10:20 Invited: Fulvio Paleari

EFFICIENT CALCULATION OF EXCITON-PHONON MATRIX ELEMENTS FOR SPECTROSCOPY AND NONEQUILIBRIUM DYNAMICS

Fulvio Paleari

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Exciton-phonon interaction is important for phenomena involving electronic excitations in weakly screened semiconductors, causing the appearance of temperature-dependent fine structures in optical spectra as well as driving exciton dynamics.
However, conceptual, numerical and computational issues have to be addressed in order to develop efficient, scalable, reliable and flexible approaches for first-principles exciton-phonon calculations.
After a brief introduction, I will first discuss how the microscopic description of exciton-phonon scattering crucially depends on the treatment of electronic screening, emphasizing that different kinds of scattering matrix elements have been proposed depending on the physical process under investigation [1, 2].
In addition, from a numerical point of view, the feasibility of first-principles calculations for large systems – such as 3D crystals – depends on the efficient interfacing of density functional perturbation theory (for phonons) with techniques based on the Bethe-Salpeter equation (for excitons).
Thus, I will present a first-principles numerical workflow for exciton-phonon calculations that allows for simulations to be run only in the irreducible part of the Brillouin zone, effectively reducing the exciton-phonon run to just a postprocessing step.
This can be achieved by exploiting lattice symmetries to efficiently rotate both exciton wavefunctions and electron-phonon matrix elements in reciprocal space. In this way, not only calculations on large systems can be attempted, but at the same time the symmetry analysis offers a way to easily obtain exciton symmetry labels and exciton-phonon selection rules. [3]
Finally, I will present examples of applications of the workflow on both 2D and 3D systems (including BN, MoS_2, $MoSe_2$, TiO_2) and for different physical processes (luminescence [4], Raman, and scattering matrix elements for Ehrenfest dynamics).

ACKNOWLEDGMENTS
Co-authors: Muralidhar Nalabothula, Matteo Zanfrognini, Davide Sangalli, Ludger Wirtz, Daniele Varsano.

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11:00-11:20 Contributed: Nicolas Baù

FIRST-PRINCIPLES REAL-SPACE EMBEDDING THEORY OF THE SUPERCONDUCTING PROXIMITY EFFECT

Nicolas Baù[1], Mitra Dowlatabadi[1], Tommaso Chiarotti[2], Massimo Capone[3], Antimo Marrazzo[3]

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[2] Department of Applied Physics and Materials Science, California Institute of Technology, Pasadena, California 91125, USA
[3] Scuola Internazionale Superiore di Studi Avanzati (SISSA), I-34136 Trieste, Italy

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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11:20-11:40 Contributed: Paolo Fachin

GALILEAN INVARIANT NON-ADIABATIC VIBRATIONAL DYNAMICS IN PSEUDO-POTENTIAL AND TIGHT-BINDING METHODS

Paolo Fachin[1], Paolo Barone[1,2], Francesco Macheda[1,3], Francesco Mauri[1]

[1] Sapienza – Università di Roma, Roma, Italy
[2] CNR-SPIN, Area della Ricerca di Tor Vergata, Roma, Italy
[3] Dipartimento di Scienze e Metodi dell'Ingegneria, Università di Modena e Reggio Emilia, Reggio Emilia, Italy

When nuclei are treated dynamically, electronic atomic orbitals acquire a nuclear-velocity-dependent phase (also known as electron-translation factor). These phases modify the effective Hamiltonians constructed from localised atomic orbitals, such as LCAO and tight-binding models as well as the non-local part of first-principles pseudo-potential Hamiltonians. Accounting for the nuclear velocity effects on electronic orbitals enables a Galilean invariant description of the first-principles nonadiabatic Ehrenfest molecular dynamics [1] - thereby removing spurious non-adiabatic couplings – and of the non-adiabatic vibrational responses, such as the Born effective charges and the force constant matrix [2,3]. In the latter case, thanks to the nuclear-velocity-dependent corrections, allelectron vibrational responses are recovered in effective models, as quantified by the fulfilment of the sum rules relating the vibrational responses to the frequency-dependent electromagnetic susceptibilities, in both the pseudo-potential [2] and the tight-binding cases [3]. Finally, tight-binding corrections are tested in the prototypical systems of metallic gapped graphene - finding excellent agreement with ab initio calculations - and of the topological time-reversal symmetry breaking Haldane model.

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11:40-12:00 Contributed: Nina Girotto Erhardt

SELF-CONSISTENCY IN ELECTRON SPECTRAL FUNCTIONS AND TRANSPORT

Nina Girotto Erhardt, Samuel Poncé

European Theoretical Spectroscopy Facility, Institute of Condensed Matter and Nanosciences, Université catholique de Louvain, Belgium

Electron spectral functions are fundamental physical quantities, crucial to understand the quasiparticle dynamics and underlying many-body interactions. Even though electron spectral functions can be directly verified experimentally, state-of-the art ab-initio implementations for the electron self-energy calculations produce unphysical results [1,2], because they are based on Migdal's theorem with the first-order one-electron and one-phonon diagram (G0D0). The G0D0 approach produces spectral functions with the wrong phonon emission onset and a slow decay inside the band gap. Apart from the well-known inability to reproduce multiple polaronic subbands in the angle-resolved photoemission spectroscopy spectra, we show how this first-order approach also produces spurious spectral features and band splittings in various 2D doped transition-metal dichalcogenides. All of these spectral artefacts then reemerge when computing optical transport properties. To address these deficiencies, we present the implementation and application of the self -consistent GD0 (scGD0) method [1,2] in the EPW software [3] and provide an alternative spectral function prediction for these materials as well as transport properties. While artefact-free, the scGD0 method yields band width and effective mass renormalizations, raising questions on its limitations.

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12:00-12:30 Invited: Jacques Desmarais

U(1)XSU(2) GAUGE SYMMETRY IN DFT AND SOLUTIONS FOR MAGNETISM

Jacques K. Desmarais

Dipartimento di Chimica, Università di Torino, Via Giuria 5, 10125 Torino, Italy

Capturing physical spin torques in noncollinear magnetic systems is a long-standing challenge in Spin Density Functional Theory (SDFT). The SDFT approach cannot rigorously include vector potentials and spin-orbit coupling. Concerning noncollinear calculations, progress in SDFT has been hindered over the last two decades by the fact that the spin torque is directly connected to the spin current — a quantity that lies outside the set of basic densities of SDFT, thus leading to spurious exchange-correlation (xc) torques in the spin dynamics. Moreover, even collinear SDFT calculations beyond the local-spin-density approximation display systemic and well-documented problems of overmagnetization.

Spin-Current DFT (SCDFT) adds to SDFT vector potentials and spin-orbit couplings. SCDFT also introduces a remarkable exact constraint, with wide-reaching consequences, that is not available in SDFT: the U(1)xSU(2) invariance of the exact xc energy functional. Here, this exact constraint allows us to extend meta-generalized-gradient approximations — in a non-empirical fashion — to include both longitudinal and transverse spin gradients [1], by means of a U(1)xSU(2) invariant electron localization function [2]. Therefore, the first-principles approach includes the full self-consistent feedback from spin-currents to treat non-perturbative spin-orbit couplings for Rashba interfaces and topologically non-trivial materials [3]. It simultaneously provides a non-empirical resolution to longstanding problems of overmagnetization [1] and removes spurious xc torques from the (adiabatic) spin-dynamics [4].

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Spectroscopy and Ultrafast Phenomena (14:30-18:00)

14:30-15:20 Keynote: Lucia Reining

EXCITONIC EFFECTS BEYOND TEXTBOOK MODELS

Lucia Reining[a,b]

[a]LSI, CNRS, CEA/DRF/IRAMIS Ecole Polytechnique, Palaiseau, France.
[b]European Theoretical Spectroscopy Facility (ETSF).

Excitation spectra of valence electrons are often dominated by interaction effects, even in the absence of strong correlation. In this talk, we start by reminding how taking into account a screened electron-hole interaction in ab initio calculations allows one to understand excitonic effects in semiconductors and insulators that go beyond textbook exciton models. We will then see examples where the electron-hole interactions can lead to surprising findings.

In the first example, we uncover a striking interplay of the direct and exchange electron-hole interactions at large momentum transfer in solid helium [1]. This interplay leads to an unexpected and very strong angular dependence of the spectra that cannot be explained by single particle matrix elements. Most importantly, a prominent excitonic peak is entirely suppressed for specific directions of momentum transfer. We show that this effect manifests dramatically near Bragg points, where even infinitesimal changes in the direction of the wave vector can switch the excitonic peak on or off. Our analysis reveals that these angular effects stem from a strong anisotropy in crystal local field effects, which modulate the electron-hole interaction by orders of magnitude. Our findings shine new light on existing experimental data and allow us to predict when such an effect will occur in other materials.

In the second example, we will discuss exotic collective excitations that may be found in low-density metals and that are of excitonic origin, in spite of perfect macroscopic screening [2]. We show that ghost modes in the irreducible polarizability and low energy modes in the dynamic structure factor cannot be captured by the standard approximations to the electron-hole Bethe Salpeter equation. Instead, one has to take into account the screening that is appropriate for fermions, and not the one that shields classical charges. Approximate vertex corrections based on time dependent density functional theory allow us to overcome this limitation and to discuss the nature of the collective modes. In particular, we highlight the importance of the short-range region of the electron-hole interaction to explain these phenomena. Finally, we will extend the study to the 2D homogeneous electron gas [3], which should be more easily accessible by experiments.

ACKNOWLEDGMENTS
This is work done in collaboration with Silvana Botti, Matteo Gatti, Jaakko Koskelo, Fatema Mohamed, and Jakob Wolff.

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15:20-15:50 Invited: Marco Garavelli

MODELLING ACCURATE NON-LINEAR ELECTRONIC SPECTROSCOPY OF PHOTOACTIVE MOLECULAR SYSTEMS IN CONDENSED PHASE

Marco Garavelli

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The use of the computer to simulate light induced events in photoactive molecular materials has given access to a detailed description of the molecular motions and mechanisms underlying the reactivity of organic and bio-organic chromophores. In parallel, simulation of transient non-linear spectral signals falling on different spectral regimes (NIR-VIS-UV-Xray) has greatly advanced in these recent years, eventually providing a mandatory tool for interpretation of experimental spectra. Thus, different computational strategies and tools can now be operated like a "virtual spectrometer" to characterize and understand the photoinduced molecular deformation and reactivity of a given dye in its operative environment, allowing for an accurate description of photochemical/photobiological processes and a rational of the corresponding photophysical properties including multi-pulses time-resolved spectroscopy.

This contribution reviews recent advances in this field, by presenting methodological developments and applications in computational photochemistry, photophysics and spectroscopy. Prototypical (bio)organic chromophores will be presented as paradigmatic test-cases [1],[2],[3],[4],[5].

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16:30-16:50 Contributed: Simone Cigagna

VARIATIONAL POLE DYNAMICS FOR MANY-BODY GREEN'S FUNCTIONS METHODS

Simone Cigagna[1], Matteo Quinzi[1], Nicola Marzari[1,2]

[1]Theory and Simulation of Materials (THEOS), École Polytechnique Fédérale de Lausanne
[2]National Centre for Computational Design and Discovery of Novel Materials (MARVEL)

We reformulate the solution of the Dyson equation as a finite-dimensional optimization over the pole positions and residues of the Green's function and self-energy. Inspired by recently developed grid-free approaches [1, 2], the formulation operates directly in the pole representation, without sampling the frequency axis. The optimization can be interpreted as an effective dynamics in the complex-frequency plane, in which poles and residues evolve toward a self-consistent configuration.

The number of poles is held fixed throughout this evolution. This avoids the pole proliferation associated with repeated algebraic Dyson updates, while providing direct control over computational cost and spectral complexity. The Dyson problem is thereby reduced to minimizing a cost function whose value and derivatives can be evaluated entirely from pole data.

We compare several choices of cost function, including the norm of the Dyson residual, variational objectives based on the Klein [3] and Luttinger–Ward [4] functionals, and modified forms designed to stabilize their stationary points as local minima. We benchmark their accuracy, convergence, and stability on the Hubbard dimer, providing a controlled comparison of grid-free optimization strategies for solving the Dyson equation.

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16:50-17:10 Contributed: Alberto Boccuni

REAL-TIME TIME-DEPENDENT CURRENT DFT IMPLEMENTATION FOR MOLECULAR AND PERIODIC SYTEMS IN THE CRYSTAL CODE

Alberto Boccuni

Department of Chemistry, University of Turin (UniTO), Turin, Italy

Interpreting electronic response properties is a central objective of materials science. Motivated by recent theorical and experimental advances in high-harmonic generation (HHG) and attosecond physics [1-3], we present a computational framework for simulating both linear and non-linear optical responses within time-dependent density-functional theory (TD-DFT). Our real-time approach directly propagates the one-particle reduced density matrix (1RDM) under an external time-dependent electric field [4], from which we obtain the time-dependent current density, $\mathbf{j}(\mathbf{r},t)$. Indeed, our method is formulated within time-dependent current-density-functional theory (TD-CDFT) [5] formalism, using a gauge in which the external electric field is represented exclusively by a time-dependent vector potential. The implementation applies to both molecular and periodic systems, but for extended systems, a current-based formulation is particularly advantageous: whereas a field-induced charge polarization occurs at the boundaries of a finite sample, the current is a bulk quantity and remains directly connected to density variations through the continuity equation [6].

Within the time-dependent generalized Kohn–Sham (TD-GKS) framework [7], the implementation is extended to hybrid exchange–correlation functionals. The inclusion of a fraction of nonlocal exact exchange is expected to improve upon adiabatic local-density-approximation (ALDA) results, particularly for the optical absorption spectra of extended systems [8]. We shall present our implementation with results for both molecules and solids, with different field shapes, highlighting the accuracy, applicability and challenges of our approach.

ACKNOWLEDGMENTS
This work is an ongoing collaboration with Jacques K. Desmarais and Stefano Pittalis, and it is currently being implemented in a developer version of the CRYSTAL code.

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17:10-17:30 Contributed: Andrea Biondini

MOLECULAR NITROGEN IN WIDE-BANDGAP NITRIDES: CONNECTING RIXS AND PHOTOLUMINESCENCE FROM FIRST PRINCIPLES

Andrea Biondini[1], Martino Silvetti[1], Saifa Amin[2], Aidan Jimenez[2], Yifeng Cao[3], Jonathan Pelliciari[3], Gabriele Grosso[2] and Marco Govoni[1]

[1]Department of Physics, Computer Science and Mathematics, University of Modena and Reggio Emilia, Italy
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Point defects in wide-bandgap semiconductors are emerging as key platforms for room-temperature single-photon emission, with applications in quantum cryptography, linear optical quantum computing, and quantum sensing [1]. Among these materials, group-III nitrides, including h-BN, w-GaN, and w-AlN, are particularly promising because their defects exhibit bright and stable emission spanning the near-infrared to the ultraviolet. However, identifying the microscopic origin of specific spectral signatures remains challenging because of the large configurational space and the overlap between emission energies.

A crucial experimental insight comes from resonant inelastic X-ray scattering (RIXS). Measurements on h-BN, w-GaN, and w-AlN reveal periodic replicas in the energy-loss spectra separated by 285 meV [2]. This energy matches the vibrational fingerprint of molecular N_2, suggesting that nitrogen molecules are trapped within the host lattice. The same vibrational periodicity is observed in donor–acceptor pair (DAP) photoluminescence [3], indicating a direct coupling between N_2 vibrations and defect-related electronic transitions.

In this work, we present a first-principles study providing a unified microscopic interpretation of the RIXS and photoluminescence observations. Using density-functional-theory-based methods, we compute formation energies, optimized geometries, vibrational modes, and optical emission properties for a set of native and carbon-related defects. Our results identify the vibration of an interstitial N_2 molecule as the origin of the characteristic energy measured by RIXS. By combining these calculations with ab initio molecular dynamics and nudged elastic band calculations, we clarify how point defects stabilize molecular N_2 within the lattice and generate the vibronic coupling responsible for the spectral replicas observed in both RIXS and photoluminescence. These findings provide a consistent microscopic interpretation of the experiments and new guidelines for identifying and engineering optically active defects in nitride-based quantum materials.

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17:30-18:00 Invited: Stefano Mocatti

A UNIFIED FIRST-PRINCIPLES APPROACH TO PHOTOCARRIER AND PHONON DYNAMICS IN PHOTOEXCITED MATERIALS

Stefano Mocatti, Giovanni Marini, Xiangzhou Zhu, Giulio Volpato, Pierluigi Cudazzo, and Matteo Calandra

Department of Physics, University of Trento, Via Sommarive 14, 38123 Povo, Italy

Interpreting ultrafast pump–probe experiments requires a predictive description of the coupled electronic and lattice dynamics of materials driven far from equilibrium by intense light pulses. In this talk, I will present a first-principles many-body framework [1], implemented in the EPIq code [2], to simulate photocarrier and phonon dynamics in semiconductors. The approach combines explicit ab initio light–matter coupling with carrier–carrier, carrier–phonon, and phonon–phonon scattering, describing also time-dependent electronic and phonon renormalizations and light-induced coherent atomic motion. The framework is implemented in a maximally localized Wannier basis, enabling gauge-consistent scattering integrals and ultradense momentum-space sampling. Using monolayer MoS_2 as a representative example, I will illustrate how the framework captures ultrafast carrier relaxation, hot-phonon dynamics, transient modifications of electronic and lattice properties, and displacive coherent atomic motion. I will then briefly discuss a recent application to photoexcited rhombohedral transition-metal dichalcogenide bilayers, showing how ultrafast photoinduced interlayer charge transfer can drive a transient reversal of the out-of-plane polarization [3].

ACKNOWLEDGMENTS
Funded by the European Union (ERC, DELIGHT, 101052708). Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Research Council. Neither the European Union nor the granting authority can be held responsible for them.

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Thursday the 27th of August 2026

Materials for Energy (9:00-12:50)

9:00-9:50 Keynote: Miguel A. L. Marques

MACHINE LEARNING-ACCELERATED DISCOVERY OF HIGH-TEMPERATURE SUPERCONDUCTORS

Miguel Marques

Research Center Future Energy Materials and Systems of the University Alliance Ruhr and Interdisciplinary Centre for Advanced Materials Simulation, Ruhr University Bochum, Universitätsstrasse 150, D-44801 Bochum, Germany

We present Alexandria [1], the largest academic database of calculated materials properties for inorganic solids, and demonstrate its application to the discovery of high-temperature conventional superconductors. The construction of Alexandria relies heavily on the massive acceleration provided by recent machine learning methods. This database serves as a training dataset for developing predictive models across multiple materials properties, such as universal machine-learning interatomic potentials or structure-property relationships. One such property is the transition temperature (Tc) of conventional superconductors. Using our trained models, we screened a chemical space of 160 million compounds, including both experimentally synthesized materials and theoretical structures, to identify promising candidates for high-Tc superconductivity. For the best candidates, we performed rigorous density-functional perturbation theory calculations to determine phonon spectra, electron-phonon coupling, and superconducting transition temperatures. This validation effort has yielded over 35,000 first-principles calculations, providing the most comprehensive computational survey of conventional superconductivity to date. This enables a systematic understanding of phonon-mediated superconductivity and allows us to establish definitive constraints on the maximum achievable Tc at ambient pressure. We conclude by discussing broader implications for the role of artificial intelligence in accelerating materials discovery and advancing fundamental understanding in materials science.

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9:50-10:20 Invited: Giorgia Fugallo (CNRS and ENS Paris)

ANHARMONICITY NEVER DIES

Giorgia Fugallo

CNRS – École Normale Supérieure Paris

The dynamics and spectral properties of a phonon are encoded in its self-energy. Anharmonic interactions renormalize phonon frequencies and generate finite spectral linewidths, leaving characteristic signatures in infrared spectra and providing the intrinsic scattering processes that constrain lattice thermal transport. In polar low-dimensional materials, coupling to the electromagnetic environment introduces an additional radiative contribution to the self-energy of infrared-active phonons. When permitted by energy, momentum, and symmetry constraints, this coupling enables photon emission and collective radiative phenomena. In this talk, I will discuss how anharmonicity constrains both thermal and radiative phenomena, limiting intrinsic heat transport and competing with photon emission [1-4]. I will further show how frequency-resolved infrared spectra, interpreted through the electrodynamic response, provide stringent tests of perturbative treatments of anharmonicity across materials of increasing structural complexity [5-6].

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11:00-11:20 Contributed: Francesca Martini

HIGH-THROUGHPUT FIRST-PRINCIPLES SCREENING OF SURFACE WORK FUNCTIONS FOR WATER SPLITTING APPLICATIONS

Francesca Martini, Matteo Calandra Buonaura

Department of Physics, University of Trento, Via Sommarive 14, 38123 Povo, Italy

The search for efficient, non-toxic, and environmentally friendly photocatalysts remains a key challenge in the field of green hydrogen production from water splitting. In this work, we perform a high-throughput computational search based on Density Functional Theory calculations using data from the AiiDA database [1], with the aim of identifying promising candidates for photocatalytic applications. We first filter out toxic compounds and restrict our selection to materials with cubic or hexagonal crystal structures, which allow for well-defined surface terminations, and with up to 12 atoms per unit cell. Among these, we retain only systems exhibiting an independent-particle band gap (properly corrected for the well-known semilocal functional deficiencies) within the visible range. For the shortlisted materials, we construct the two most common surface terminations and compute their work functions, which serve as key descriptors for photocatalytic activity. Candidate materials for hydrogen evolution are identified based on the alignment of their bottom conduction with the Standard Hydrogen Electrode, while anodic suitability is assessed through the position of the valence band maximum relative to the oxidation potential. The resulting set of materials includes both well-known photocatalysts and previously unexplored compounds, providing a curated pool of candidates for further investigation. We also assess the presence of critical raw materials, highlighting potential trade-offs between performance and sustainability.

ACKNOWLEDGMENTS
We acknowledge support from the project Produrre Idrogeno in Trentino – H2@TN (PATTrento).

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11:20-11:40 Contributed: Andrea Droghetti

ELECTRONIC CORRELATIONS IN NANODEVICES UNDER BIAS

Andrea Droghetti

Department of Molecular Sciences and Nanostructures, Ca' Foscari University of Venice, Italy

Understanding how electronic correlations evolve under non-equilibrium conditions is one of the outstanding challenges in condensed matter physics. While remarkable progress has been made in describing correlated quantum materials in equilibrium, our predictive understanding of how many-body interactions influence transport in devices under finite bias remains rather limited. Here, we present a first-principles framework that combines density functional theory (DFT), non-equilibrium Green's functions (NEGF), and dynamical mean-field theory (DMFT), enabling predictive simulations of correlated quantum transport in nano-devices under realistic operating conditions [1-5]. The approach is applicable to a broad class of magnetic materials and heterostructures. Our results uncover a non-equilibrium many-body regime in the two-dimensional van der Waals magnet Fe_4GeTe_2 in which an applied voltage drives strong electron-electron scattering, creating hot correlated electrons [6,7]. In this regime, electronic correlations are not merely perturbed by the bias—they are actively reshaped by it, producing distinctive spectroscopic and transport signatures accessible to experiments. Extending the formalism to spin-transfer torque further reveals how non-equilibrium electronic correlations can modify current-driven spin dynamics. More broadly, these results establish voltage as a means of controlling many-body electronic states and open the way to predictive first-principles design of correlated quantum devices.

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11:40-12:00 Contributed: Michele Bagaglini

TWISTRONIC CONTROL OF SHIFT CURRENT IN MULTILAYER MOIRÉ SYSTEM

Michele Bagaglini[1,2], Cesare Tresca[2], Federico Bisti[1], and Gianni Profeta[1, 2]

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The bulk photovoltaic effect in non-centrosymmetric materials provides an alternative mechanism for the conversion of light into a current response compared to p–n junctions. Among its various contributions, the shift current is particularly attractive because it is governed by the geometric properties of electronic wavefunctions and can generate large photocurrents in low-dimensional materials. Here, we investigate the evolution of the shift current response in mono-, bi-, and trilayer H-MoS2, as well as in twisted moiré bilayers and trilayers. To describe large moiré supercells we develop a Slater–Koster tight-binding model parametrized from first-principles calculations. The resulting electronic structures and shift-current responses are compared with density functional theory calculations and Wannier-interpolated results to verify the accuracy of the approach. The model accurately reproduces the electronic structure near the band edges and captures the main spectral features of the shift current conductivity. We show that twisting breaks the crystal symmetry and activates additional conductivity tensor components that are forbidden in untwisted structures, leading to new tunable in-plane photocurrent components. Analysis of the shift distance reveals a direct connection between the twist-induced modification of the electronic wavefunctions and the increase of the nonlinear response. Our results establish the twist angle as an effective parameter for engineering shift current generation in multilayer transition-metal dichalcogenide base systems and demonstrate that tight-binding approaches provide a practical route for exploring nonlinear optical phenomena in large-scale moiré materials beyond the limits of conventional first-principles calculations.

ACKNOWLEDGMENTS
C. T. and F. B. acknowledge financial support under the National Recovery and Resilience Plan (NRRP), Mission 4, Component 2, Investment 1.1, funded by the European Union-NextGenerationEU- Project Title "Symmetry-broken HEterostructurEs for Photovoltaic applications-SHEEP" – CUP B53D23028580001 – Grant Assignment Decree No. 1409, adopted on 14 September 2022 by the Italian Ministry of Ministry of University and Research (MUR).

12:00-12:30 Invited: Paolo Pegolo

COUPLED HEAT AND CHARGE TRANSPORT FROM EQUILIBRIUM MOLECULAR DYNAMICS

Paolo Pegolo

Laboratory of Computational Science and Modeling, Institut des Matériaux, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

Understanding and controlling the coupled transport of heat and charge is central to the design of efficient thermoelectric materials and solid-state ionic conductors. Yet predicting transport coefficients from equilibrium molecular dynamics remains challenging, requiring long simulations and robust statistical tools, all the more so for the off-diagonal coefficients that govern thermoelectric phenomena. I will present a unified framework based on the spectral analysis of current time series, enabling the accurate computation of the full Onsager matrix – diagonal and off-diagonal elements alike – from a single statistical model. I will briefly survey applications ranging from molten salts and liquid water to the Li_3PS_4 and Li_3ClO solid electrolytes and SiGe thermoelectric alloys, where these tools help disentangle the interplay of anharmonicity, ionic diffusion, and mass disorder in heat transport. I will conclude with an outlook on the ionic thermoelectric effect in water under the extreme pressure-temperature conditions of ice-giant interiors, where self-dissociation turns water into an ionic conductor and coupled heat-charge transport remains largely uncharted – precisely the regime where access to the full Onsager matrix becomes essential.

Machine Learning in Condensed Matter Physics (14:00-17:30)

14:00-14:50 Keynote: Paul Erhart

ACCELERATING ADVANCED SIMULATIONS BY MACHINE LEARNING: FROM MODELS TO INSIGHT

Paul Erhart

Chalmers University of Technology, Department of Physics and Astronomy, Gothenburg, Sweden

The widespread adoption of machine learning techniques is currently leading to an dramatic expansion of the capabilities of atomic scale simulations. Machine-learned interatomic potentials (MLIPs) are at the center of this development. A large variety of MLIP architectures has been introduced over the last decade or so that cannot only map the ground state energy landscapes predicted by electronic structure calculations. They also form the basis for so-called foundational MLIPs that can promise to provide a basic description of chemistries across the entire periodic table.

In this contribution I will try to provide a concise summary of the basic architectural principles and the implications for not only the accuracy but the computational speed that can be achieved. I will then focus on a particular class of MLIPs, namely neuroevolution potential (NEP) models [1]. I will show how this architecture can be expanded to become charge aware while maintaining very high computational efficiency. The resultant qNEP models enable simulations of 100k atoms for tens of ns per day on a single GPU [2].

These models can be expanded further to enable spectroscopic studies, e.g., the prediction of defect line shapes [3], dielectric functions as well as infrared and Raman spectra [4], and also extended Hamiltonians that couple, e.g., matter and cavity degrees of freedom [5]. Several of these applications require sampling the polarization (or dipole in a finite system) and susceptibility (or polarizability), respectively, which is enabled by tensorial NEP (TNEP) models [6].

Finally, I will demonstrate how these approaches can even be extended to model the position and composition dependence of the electronic dielectric function, providing access to finite temperature optical properties in complex systems.

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14:50-15:20 Invited: Volker Deringer

15:20-15:40 Contributed: Sita Schoenbauer

MACHINE-LEARNED FORCE FIELDS FOR LATTICE DYNAMICS AT COUPLED-CLUSTER LEVEL ACCURACY

Sita Schönbauer

Institute of Theoretical Physics, Technical University of Vienna, Wiedner Hauptstrasse 8−10, 1040 Vienna, Austria

We investigate machine-learned force fields (MLFFs) trained using MACE [1,2] on approximate density functional theory (DFT) and coupled cluster (CC) level potential energy surfaces for the carbon diamond and lithium hydride solids. We assess the accuracy and precision of the MLFFs by calculating phonon dispersions and vibrational densities of states that are compared to experimental and reference ab initio results. To overcome limitations from long-range effects and the lack of atomic forces in the CC training data, a delta-learning approach based on the difference between CC and DFT results, as well as a charge-aware MLFF approach, is explored. Compared to DFT, MLFFs trained on CC theory yield higher vibrational frequencies for optical modes, agreeing better with the experiment. [3]

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16:20-16:40 Contributed: Andrea Baldanza

ANHARMONICITY AND STRUCTURAL PHASE TRANSITION IN LAALO3 USING SSCHA AND ML FORCE FIELDS

A. Baldanza[1], L. Monacelli[1]

[1]La Sapienza Università di Roma

Lanthanum Aluminate (LaAlO3) is an insulating perovskite that has attracted significant interest from both the scientific and technological communities[1]. It is widely used as a substrate for the growth of thin superconducting films[2], and it has gained particular attention due to the remarkable properties emerging at the LaAlO3/SrTiO3 interfaces[3], including the formation of a two-dimensional electron gas[4, 5], and the appearance of low-temperature superconductivity[6]. Recently, THz pump-probe experiments have also revealed strong non-linear lattice dynamics in the bulk, including the parametric excitation of Raman-active phonons[7]. Despite the intense interest in the LaAlO3, an accurate ab initio description remains challenging due to the strong anharmonicity, which drives a structural phase transition from a low-symmetry rhombohedral phase (R3c) to a high-symmetry cubic phase (Pm3m) at ∼ 800 K[8, 9]. Capturing these strong anharmonic and quantum nuclear effects in the bulk is therefore a crucial prerequisite both to understand its non-equilibrium dynamical response, and to better characterize the emerging physics of LaAlO3-based interfaces. In this poster, we present an ab initio study of bulk LaAlO3, based on Stochastic Self-Consistent Harmonic Approximation (SSCHA)[10–15], a non-perturbative method capable of incorporating full anharmonicity and quantum nuclear fluctuations. To overcome the high computational cost associated with the stochastic evaluation of ionic forces, we employ a machine-learning force field based on NequIP [16], trained on hundreds of DFT configurations. This approach allows us to perform extensive SSCHA simulations over a wide range of temperatures and pressures at minimal computational cost. After accurately reproducing the experimental thermal expansion, we investigate the instabilities driving the structural phase transition, analysing the effects of IIIrd and IVth orders in the SSCHA Free Energy Hessian in both the cubic and rhombohedral phases.

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16:40-17:00 Daniela Mangano (Contributed)

NONADIABATIC POLARON DYNAMICS FROM MACHINE-LEARNED HOPPING TRAJECTORIES

Daniela Mangano[a,b], Luca Leoni[b], Zhong-Fei Xu[c,d,e], Li-Min Liu[d], Cesare Franchini[a,b]

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The formation of small polarons through charge trapping is a widespread phenomenon in transition metal oxides, and the motion of these quasiparticles plays a crucial role in a broad range of processes, including charge transport, optical absorption, and chemical reactivity. Because polarons significantly influence photocatalytic activity and other photoinduced phenomena, a detailed understanding of the mechanisms governing their formation, excitation, and dynamics is essential for the rational design and optimization of functional materials. In this context, nonadiabatic effects must be explicitly considered, as they describe the interplay between electronic and nuclear degrees of freedom beyond the Born–Oppenheimer approximation. The coupling between fast electronic dynamics and slower lattice vibrations controls energy transfer, charge-carrier relaxation, and hopping processes, making nonadiabatic interactions a key ingredient for a realistic description of polaron dynamics and photoinduced phenomena.
In this study we examine polaron hopping in rutile TiO_2, both in the bulk and at the (110) reduced surface, together with bulk MgO. We use machine learning molecular dynamics trajectories, which allows us to obtain a richer sampling of hopping events. Then, in the framework of decoherence induced surface hopping we run nonadiabatic molecular dynamics simulations to elucidate how different types of polaron hopping distinctly influence the excited state dynamics of the materials. We investigate the relationship between the dynamic behavior of nonadiabatic couplings and polaron hopping events and examine how these processes correlate with the time evolution of the polaronic energy bands. Furthermore, we evaluate the charge carrier lifetime in systems hosting electron and hole polarons, comparing the results for different temperatures.

ACKNOWLEDGMENTS
This research was funded by the Austrian Science Fund (FWF) project TACO.

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17:00-17:30 Invited: Andrea Grisafi

MACHINE LEARNING OF ELECTRONIC CHARGE DENSITIES IN THE SIMULATION OF ELECTROCHEMICAL INTERFACES

Andrea Grisafi

Physicochimie des Electrolytes et Nanosystèmes Interfaciaux (PHENIX), Sorbonne Université, CNRS, F-75005 Paris, France

Machine-learning methods are playing a prominent role in the atomistic simulation of materials. When it comes to electrochemical systems, however, the effective implementation of these approaches presents unique challenges. Notably, the presence of a heterogeneous interface between an electrode and an electrolyte solution under an applied electric bias requires predicting complex long-range interactions that drive the dynamics of the system at the nanoscale. In this context, I will first introduce a machine-learning model suitable to predict the electron density of a system [1] and show how its combination with long-range atomistic features [2] can be used to account for nonlocal electronic charge effects [3], as well as nonlocal electric-field responses [4]. I will then show how to take advantage of similar models to simulate the long-range electrostatics of model ionic capacitors under an applied voltage, matching the accuracy of density-functional QM/MM methods while allowing for a thermally relaxed description of the electrical double layer [5]. I will conclude discussing future directions for the adoption of electron-density models towards a complete description of electrochemical charging

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Friday the 28th of August 2026

Magnetism, superconductivity and topology (9:00-12:30)

9:00-9:50 Keynote: Maia Vergniory

FROM THEORY TO MATERIALS: THE SEARCH FOR TOPOLOGICAL QUANTUM MATTER

Maia G. Vergniory[1,2]

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The discovery of topological phases has profoundly changed our understanding of quantum materials. What began as a theoretical framework describing exotic electronic states has evolved into a powerful paradigm for predicting, classifying, and discovering real materials with novel quantum properties. Today, topology provides a unifying language that connects symmetry, electronic structure, magnetism, and strong correlations across a wide range of material platforms. In this talk, I will discuss how advances in theoretical condensed matter physics have transformed the search for topological quantum matter from a collection of isolated examples into a systematic materials-discovery enterprise. I will present the development of symmetry- based approaches, including Topological Quantum Chemistry, that enable the identification of topological materials directly from their crystal structures and electronic bands. These methods have revealed that topological phenomena are far more prevalent in nature than previously imagined, opening new opportunities for both fundamental science and future technologies. I will then highlight recent developments at the frontier of the field, where topology intertwines with magnetism, chirality, and electronic correlations. These interactions give rise to new quantum states, including magnetic topological phases, altermagnets, correlated topological materials, and unconventional quasiparticles that challenge traditional classifications of matter. Through selected examples, I will illustrate how the synergy between theory, computation, and experiment is accelerating the discovery of materials with unprecedented electronic and magnetic functionalities.

9:50-10:20 Invited: Dario Fiore Mosca

EFFECT OF DOPING ON DOUBLE PEROVSKITES: FROM POLARONS TO HIDDEN ORDERS

Dario Fiore Mosca

University of Vienna

Spin-orbit-entangled 5d double perovskites host a rich landscape of high-rank multipolar "hidden" orders whose local order parameters evade conventional experimental probes [1]. In the $5d^2$ osmate Ba2CaOsO6, a ferro-octupolar phase breaks time-reversal symmetry while leaving the cubic structure and dipole moments unobservable [2]. Substituting Ca with Na pushes the system toward the $5d^1$ limit, progressively suppressing this order [3].

In this talk I will show how charge doping provides a controllable handle on intersite multipolar exchange. The key insight is that dopant charges in Ba2Ca1-xNaxOsO6 form small polarons with $5d^1$ electronic configuration embedded within the $5d^2$ matrix [4]. Using a fully ab initio approach that combines density functional theory (DFT)+dynamical mean-field theory with the force-theorem Hubbard-I method, alongside DFT+U and mean-field calculations, we compute the mixed intersite exchange between Jeff = 3/2 polarons and Jeff = 2 ions and find that the dominant octupolar coupling reverses sign, from ferro- to antiferro-octupolar, at the polaronic bond. This reversal produces a localized antiferro-octupolar polaron embedded within the broader ferro-octupolar phase. We trace this effect to the distinct representations of the one-electron t2g operators in the one- and two-electron manifolds, a mechanism that accounts quantitatively for both the suppression of the multipolar order and the doping dependence of the ordering temperature [5].

More broadly, these findings establish that by locally reshaping the magnetic landscape, charge doping via small polarons can be viewed as a tool for engineering novel quantum phases in spin-orbit-coupled materials.

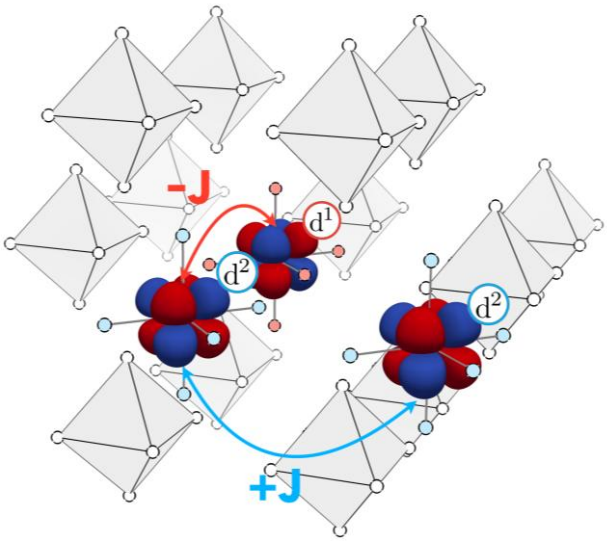

FIG: The figure shows the hidden octupolar order changing orientation on the $5d^1$ site, as a consequence of the dominant exchange interaction J flipping sign due to polaron localization.

ACKNOWLEDGMENTS
I would like to thank the co-authors: Lorenzo Celiberti, Cesare Franchini and Leonid V. Pourovskii.

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11:00-11:20 Contributed: Luigi Camerano

MULTIFERROIC ALTERMAGNETISM AND MAGNETO-ORBITAL EXCITATIONS IN MONOLAYER VCl_3

Luigi Camerano[1,2], Adolfo Otero Fumega[3], Jose Lado[3], Alessandro Stroppa[2] and Gianni Profeta[1,2]

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Van der Waals monolayers featuring magnetic states provide fundamental building blocks for artificial quantum matter. In this contribution I will present the emergence of a symmetry broken multiferroic ground state featuring magneto-orbital excitations and nematic d-wave altermagnetism in monolayer VCl3 [1-4]. All this physics arises from a pure electronic symmetry breaking ultimately stabilizing an antiferro-orbital order ground state showing the emergence of an electronic polarization. Recent experimental evidence reports signatures of symmetry breakings and ferroelectricity combined with 2D magnetism, establishing monolayer VCl3 as a novel 2D multiferroic driven by orbital ordering.

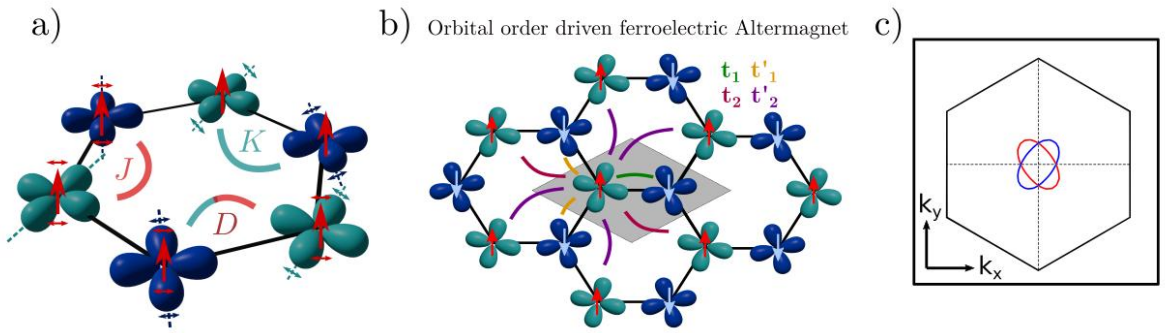

Fig. 1 a) Schematics of the model describing monolayer VCl3, reprinted from ref. [3]. The system shows magnetic coupling (J), orbital coupling (K) and magneto-orbital coupling (D). b) When antiferro-orbital ordering is coupled with antiferromagnetism, an altermagnetic phase with non-zero polarization emerges. c) The Fermi surface of this multiferroic states has a nematic d-wave symmetry, reflecting the electronic symmetry breaking of the monolayer VCl3. Images b) and c) are reprinted from ref [4].

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11:20-11:40 Contributed: Johanna Paulina Carbone

POLARON-INDUCED TRANSFORMATION OF MAGNETIC EXCHANGE IN 2D-MAGNETS

Johanna P. Carbone

Faculty of Physics and Center for Computational Materials Science, University of Vienna, Austria

Two-dimensional magnetic materials have emerged as a versatile platform for exploring low-dimensional magnetism and its control at the atomic scale, with promising applications in spintronics and next-generation information storage technologies. At the same time, charge localization phenomena such as polarons, quasiparticles formed by the coupling of excess charge carriers with lattice distortions, are known to strongly influence the electronic, optical, and chemical properties of polarizable semiconductors [1]. However, polaron physics in 2D systems remains largely unexplored, with only a few studies (e.g., in monolayer $CoCl_2$ [2,3]) and limited attention to their interplay with magnetism.

In this work, we explore the interaction between polarons and magnetism in monolayer $MnPS_3$, a prototypical two-dimensional antiferromagnet. Using first-principles calculations, we show that electron polarons can serve as an effective means to alter the size and nature of magnetic exchange interactions. In particular, polaron formation is found to break the magnetic symmetry and locally enhance exchange couplings and their anisotropic character with respect to the underlying magnetic texture [4]. Our findings point to emergent higher-order magnetic interactions beyond pairwise exchange driven by charge localization. These results identify polaron engineering as a promising strategy for locally tuning magnetism in two-dimensional materials, opening new possibilities for externally controlled and functional manipulation of magnetic textures at the atomic scale.

ACKNOWLEDGMENTS
Special thanks to Jakob Baumsteiger and Cesare Franchini to their essential contributions to this work, and to Eduardo Mendive Tapia and Gustav Bihlmayer for valuable discussions.

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11:40-12:00 Contributed: Srdjan Stavric

EMERGENT NONRECIPROCITY IN A P-WAVE MAGNET NII2: DESCRIPTORS FOR DATA-DRIVEN FUNCTIONAL MATERIALS

Srdjan Stavric

Vinca Institute of Nuclear Sciences

Using first-principles calculations and symmetry analysis, we investigate the nonlinear optical transport of van der Waals NiI2, which hosts coexisting spin-spiral multiferroicity and p-wave magnetism [1]. We show that second-order photogalvanic responses uniquely disentangle these intertwined phases [2], identifying key symmetry-based features for the data-driven screening of nonreciprocal transport. Magnetically-induced inversion-symmetry breaking activates a substantial linear shift current, outperforming conventional bulk oxide ferroelectrics. Conversely, circularly polarized light drives a large charge injection current via helicity-selective transitions between spin-split bands, fingerprinting the p-wave spin texture. In time-reversal-broken, odd-period spin spirals, we unveil a linear injection current arising from asymmetric band dispersion. This response mirrors the T-odd nonreciprocal transport reported in multiferroic EuO [3] but exhibits distinct directional constraints. Finally, we predict pure spin photocurrents whose orthogonal trajectories can be deterministically switched via light polarization. Our work provides a framework for symmetry-broken nonlinear optical probing of p-wave magnetism, thus establishing the physical descriptors required to accelerate the data-driven engineering of functional materials for all-optical spintronics.

ACKNOWLEDGMENTS
[1] COST action DAEMON: Data-driven applications towards the engineering of functional materials
[2] Ministry of Science, Technological Development, and Innovation of Serbia and Ministry of Foreign Affairs of Italy for the bilateral project "Van der Waals Heterostructures for Altermagnetic Spintronics"

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12:00-12:30 Invited: Zeila Zanolli

DENSITY FUNCTIONAL BOGOLIUBOV-DE GENNES THEORY FOR SUPERCONDUCTORS

Zeila Zanolli

University, Debye Institute for Nanomaterials Science and European Theoretical Spectroscopy Facility

Superconductors are materials that conduct electrical current without resistance below a critical temperature due to a mechanism that pairs electrons into coherent quantum states. Their unique properties enable transformative technologies ranging from particle accelerator magnets and MRI scanners to emerging quantum technologies such as qubits and ultrasensitive detectors. At present, all large-scale and commercial applications rely on conventional superconductors, in which the pairing mechanism is well understood and described within the Bardeen–Cooper–Schrieffer (BCS) framework. However, these materials operate only at extremely low temperatures, typically between 1 and 10 K, requiring bulky and energetically expensive cryogenic infrastructures. This not only limits widespread deployment but also raises significant sustainability concerns and hinders miniaturization and portability. High-temperature superconductors offer a possible solution. However, the microscopic mechanism driving high-temperature superconductivity goes beyond BCS theory and remains unknown. Without a predictive understanding of the pairing mechanism, it is impossible to rationally design new superconducting materials with elevated critical temperatures beyond known families.

With my group, we target this long-term ambitious project. We developed a theoretical framework and code implementation for the simultaneous solution of the superconducting (Bogoliubov-de Gennes, BdG) and electronic (Density Functional Theory, DFT) problems [1]. Our method, SIESTA-BdG, is implemented in SIESTA, a first-principles DFT code for material simulations. Our unified approach describes both conventional and unconventional superconducting phases, and enables a description of inhomogeneous superconductors, heterostructures, and proximity induced superconductivity [2]. We demonstrate the validity, accuracy, and efficiency of SIESTA-BdG by computing physically relevant quantities (superconducting charge density, band structure, superconducting gap features, density of states) for conventional singlet (Nb, Pb) and unconventional (FeSe) superconductors. We find excellent agreement with experiments. SIESTA-BdG forms the basis for modeling quantum transport in superconducting devices, and to bridge DFT with Dynamical Mean-Field Theory (DMFT) to model high-temperature superconductivity in strongly correlated electron systems.

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ABSTRACTS OF POSTERS

Session 1 – Wednesday the 26th of August 2026 – 18:00-19:30

Barducci Marco	Machine Learning Polaron Dynamics in lithium anode Li4Ti5O12
Bastos Vinicius Alves	Probing Bound Excitons in Monolayer SnS: A First-Principles Study
Baumsteiger Jakob	Understanding Magnetic Anisotropy in Co doped Barium Hexaferrite
Bhumla Preeti	First-Principles Investigation of Phonon Anharmonicity and Low Lattice Thermal Conductivity in Matlockite-Type Ternary Chalcogenides
Bodo Filippo	Extending Local Vibrational Mode Theory to Periodic Systems
Borghi Andrea	Interplay between vibrational and electronic infrared spectrum in Haldane model nanoribbons
Brangi Pietro Nicolò	Electron-Phonon Coupling in Magnetic Materials Through Wannier Function Interpolation
Caldarelli Giovanni	Effective single particle picture for anharmonic lattice dynamics
Choudhury Amarjyoti	Switchable Chern number in van der Waals heterostructures
Damian Niccolò	Effects of exciton-phonon coupling on optical spectra of TMDs via cumulant approach
De Simone Andrea	F-sum rule in Bethe-Salpeter, (screened) Hartree-Fock, Hybrid-DFT approaches
Gelli Andreha	Implementing tools to explore reaction pathways for periodic systems in CRYSTAL
Giannessi Federico	Secondary electron emission in multilayer systems
Gottardi Lorenzo	Benchmarking Excited-State Methods for Quantum Defects: The Role of Electronic Localization
Grasselli Federico	Long-range electrostatics in atomistic machine learning: a physical perspective
Kataria Anshu	Hidden order investigation in 5d2 osmates: A MuSR study

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MACHINE LEARNING POLARON DYNAMICS IN LITHIUM ANODE $LI_4TI_5O_{12}$

Marco Barducci[1], Luca Leoni[1], Cesare Franchini[1,2]

[1]Department of Physics and Astronomy "Augusto Righi", University of Bologna, [2]Faculty of Physics and Center for Computational Materials Science, University of Vienna

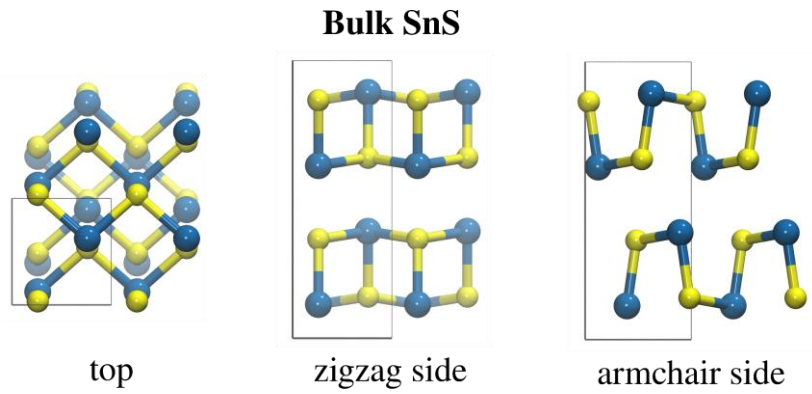
Polarons play a central role in mediating Li-ion diffusion in the $Li_4Ti_5O_{12}$ (LTO) anode. The presence of polarons reduces the energy barrier for Li-ion diffusion and influences both electronic and ionic mobility. However, mobility estimation remains a significant challenge for purely ab initio methods, since the relevant timescales exceed by orders of magnitude those accessible via ab initio molecular dynamics. Machine learning interatomic potentials (MLIPs) provide a promising alternative, combining the accuracy of first-principles methods with substantially reduced computational cost, thus enabling simulations on the nanosecond timescale. In this work, we employ the recently developed MLIP architecture LEOPOLD (Learning of Polaron Dynamics) to estimate the mobility of a single polaron in bulk LTO. This represents a crucial first step toward a broader understanding of polaron dynamics and their impact on Li-ion transport in LTO for battery applications.

PROBING BOUND EXCITONS IN MONOLAYER SNS: A FIRST-PRINCIPLES STUDY

Vinicius Alves Bastos[1],*, Fulvio Paleari[2], Eleonora Luppi[3], and Alice Ruini[1,2]

[1]FIM Department, UNIMORE – Modena, Italy (*vinicius.alvesbastos@unimore.it), [2]CNR-Nano – Modena, Italy, [3]LCT, Sorbonne Université – Paris, France

Monolayer SnS is a material of the class of group-IV monochalcogenides, which, unlike the more studied dichalcogenides, does not form a hexagonal lattice but an anisotropic orthorhombic one. They have gained increased attention for exhibiting multiferroic order up to above room temperature [1] and gigantic second-harmonic generation (SHG) response [2]. Here we have performed a first-principles study of bound excitons in monolayer SnS, computed using GW-BSE [3]. The optical response in this system results from competing electronic transitions involving two different valleys. We show how valley-selection control can be achieved using linearly polarized light along either the zigzag or the armchair direction, a consequence of the system anisotropy. In this way, we turn on and off the bright excitons corresponding to the different valleys. We also show that the energy of the two bright excitons decreases with increasing number of SnS atomic layers due to the change in the intervalley quasiparticle energy difference. All this has potential applications in valleytronics [4]. Finally, given the importance of polarisation-dependent bright excitons in this system, we investigate the excitonic effects in the nonlinear SHG response of monolayer SnS, not yet addressed in the literature.



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UNDERSTANDING MAGNETIC ANISOTROPY IN CO DOPED BARIUM HEXAFERRITE

Jakob Baumsteiger

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M-type hexaferrites are widely used permanent magnetic materials with important technological applications. They are also promising for next-generation microwave devices, such as optimized circulators for future telecommunication systems. A promising pathway to adapting the operating frequency of unbiased M-type hexaferrite circulators is to tune the magnetocrystalline anisotropy energy (MAE) through cation substitution. Although the effects of cation substitution on the magnetic properties of M-type hexaferrites have been studied extensively, largely through experiment, the microscopic mechanisms governing these changes remain poorly understood. Here, we investigate cobalt-doped barium hexaferrite, $BaFe_{12-x}Co_xO_{19}$, at doping concentrations of x=0 and x=0.5 using density functional theory (DFT). We find that Co substitution is energetically most favorable at the 2b and 12k sites, while thermal occupation favors the 12k site above approximately 20 K. For the undoped compound, we calculate an MAE of 335 kJ/m^3 and confirm that it is dominated by contributions from the 2b and 12k sublattices. We further show that the MAE of the doped system depends strongly on the substitution site, with two of the five possible Co sites inducing an easy-plane magnetic ground state. Finally, we demonstrate that Co substitution at the octahedral 2a site stabilizes an occupied localized d_{z^2} orbital, thereby weakening the easy-plane anisotropy.

FIRST-PRINCIPLES INVESTIGATION OF PHONON ANHARMONICITY AND LOW LATTICE THERMAL CONDUCTIVITY IN MATLOCKITE-TYPE TERNARY CHALCOGENIDES

Preeti Bhumla and Silvana Botti

Research Center Future Energy Materials and Systems of the University Alliance Ruhr and Interdisciplinary Centre for Advanced Materials Simulation, Faculty of Physics and Astronomy, Ruhr University Bochum, Bochum, Germany

We report a first-principles investigation of the phonon and thermal transport properties of the Matlockite-type ternary chalcogenides RbNaS, CsNaS, CsNaSe, and CsNaTe, identified as low-lattice-thermal-conductivity candidates through high-throughput screening (Li, Hu, Yang, JACS 2022). Using density functional theory and third-order interatomic force constants, we investigate the lattice thermal conductivity (κ_l), mode-resolved Grüneisen parameters, and phonon lifetimes. Representative results obtained for RbNaS and CsNaS confirm their dynamical stability and reveal pronounced phonon anharmonicity at low frequencies, with Grüneisen parameters reaching approximately 4-5 for CsNaS and ~3.5 for RbNaS in the acoustic branches. At 300 K, both

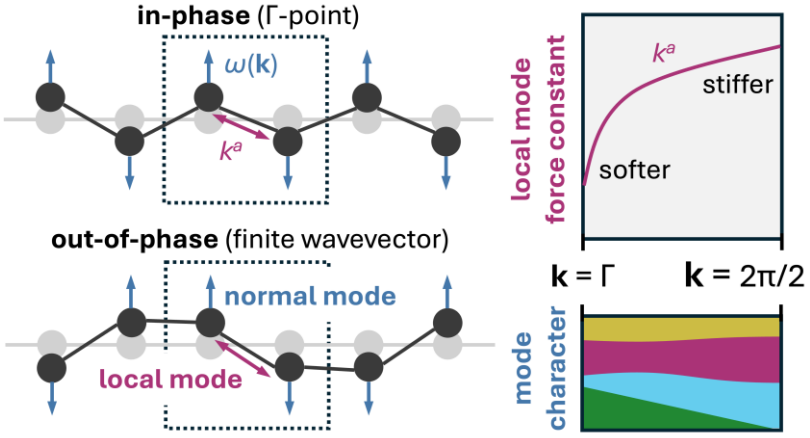
compounds exhibit low and anisotropic lattice thermal conductivity: CsNaS has $\kappa_x \approx 0.48$ and $\kappa_z \approx 0.18$ W m^{-1} K^{-1}, while RbNaS has $\kappa_x \approx 0.85$ and $\kappa_z \approx 0.35$ W m^{-1} K^{-1}. Compared with RbNaS, CsNaS exhibits stronger anharmonicity and lower κ_L, consistent with enhanced rattling of the weakly bonded Cs cations in the Matlockite framework. Phonon lifetime analysis further supports this mechanism, revealing relatively long-lived acoustic phonons and short-lived optical phonons that promote strong phonon scattering and suppress heat transport. Ongoing calculations on CsNaSe and CsNaTe will enable a systematic comparison of lattice dynamics and thermal transport across the Matlockite family.

EXTENDING LOCAL VIBRATIONAL MODE THEORY TO PERIODIC SYSTEMS

Filippo Bodo

Dipartimento di Chimica, Università di Torino, via Giuria 5, 10125 Torino, Italy

The Local Vibrational Mode Theory (LVMT), in its molecular formulation, has traditionally offered a framework capable of decoding the bond strength and intermolecular interaction information contained in vibrational spectroscopy data, offering insights on reactivity mechanism and structural response during reactions. Here we present the extension of the LVMT formalism to periodic systems for arbitrary wave-vectors throughout the Brillouin Zone. Besides providing a quantity measurement of the intrinsic strength of interatomic interaction, in the form of a force constant, the LVMT provides another key tool in characterization of the normal mode (CNM). The CNM decomposes, through an adiabatic connection scheme, the delocalized normal modes in terms of their internal coordinate (bonds, angles, and dihedrals) contribution. By resolving the normal modes in internal coordinate contribution the LVMT framework enables the interpretation of phonon dispersion relation in terms of chemically meaningful interatomic interactions and structural motifs capable of providing direct insight on the microscopic origin of phonon behavior in periodic systems.



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INTERPLAY BETWEEN VIBRATIONAL AND ELECTRONIC INFRARED SPECTRUM IN HALDANE MODEL NANORIBBONS

Andrea Borghi[1], Paolo Fachin[1], Francesco Macheda[2], Paolo Barone[1] and Francesco Mauri[1]

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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
We acknowledge the MORE-TEM ERC-SYN project, grant agreement no. 95121.

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ELECTRON-PHONON COUPLING IN MAGNETIC MATERIALS THROUGH WANNIER FUNCTION INTERPOLATION

Pietro Nicolò Brangi, Giovanni Marini, Matteo Calandra

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Magnetic materials, ranging from traditional collinear ferromagnets to ones hosting complex, non-collinear spin structures, are the cornerstones of next-generation spintronics, low-power memory devices, and quantum information processing. In these systems, the interaction between electrons and lattice vibrations (phonons) fundamentally dictates spin-relaxation times, carrier mobility, and thermal transport, while also allowing for the excitation of chiral phonons driven by non-adiabatic effects. However, accurately modeling electron-phonon coupling (EPC) in magnetic phases remains a formidable challenge due to the massive computational cost of dense Brillouin-zone (BZ) sampling.

To overcome this bottleneck, we develop an implementation that generalizes Wannier Function (WF) interpolation of EPC to the case of magnetic materials. Our approach handles both collinear spin-polarized systems and fully relativistic non-collinear magnets that require spinor wavefunctions. We implement the rotation of the derivative of the Kohn-Sham potential and of the dynamical matrix in the case of non collinear magnets, exploiting the symmetries of the system, allowing for the treatment with the EPIq software [1]. By projecting the EPC matrix elements onto a localized real-space basis, our code enables highly efficient and computationally inexpensive interpolation on ultra-dense momentum grids, needed to accurately converge adiabatic and non-adiabatic phonon dispersions.

We demonstrate the capabilities of our method by computing the spin-resolved phonon linewidth in a prototypical collinear magnet such as Fe, and well-converged adiabatic phonon dispersions together with non-adiabatic frequency shifts and phonon angular momenta across the whole BZ in the case of the noncollinear magnet Mn3Pt.

Our work paves the way for future developments in the fields of ultrafast magnetization, magnetic transport and magnon-phonon interaction.

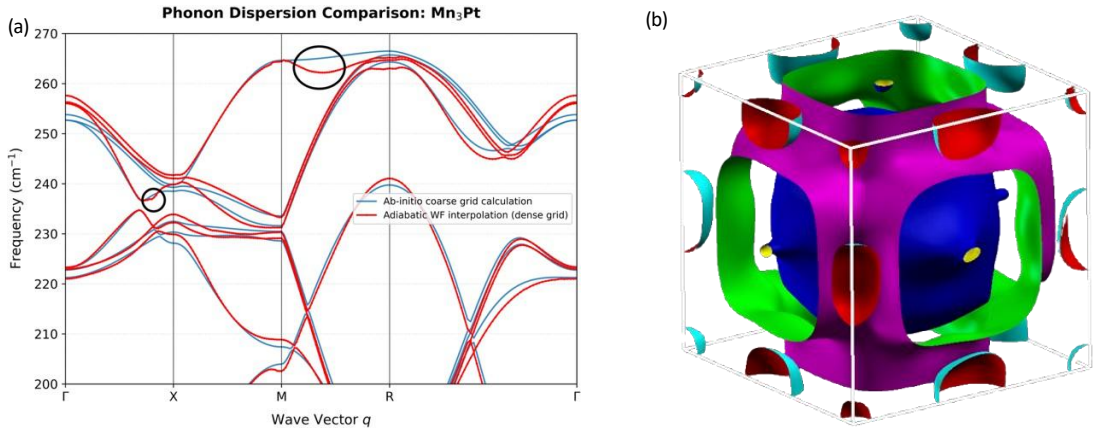

Fig. 1: (a) Comparison between ab-initio phonon dispersion in Mn3Pt computed on a coarser k-grid and the WF interpolated dispersion on a denser mesh.
One can see the appearance of noticeable Kohn-anomalies due to Fermi Surface nesting; (b) Fermi surface of Mn3Pt.

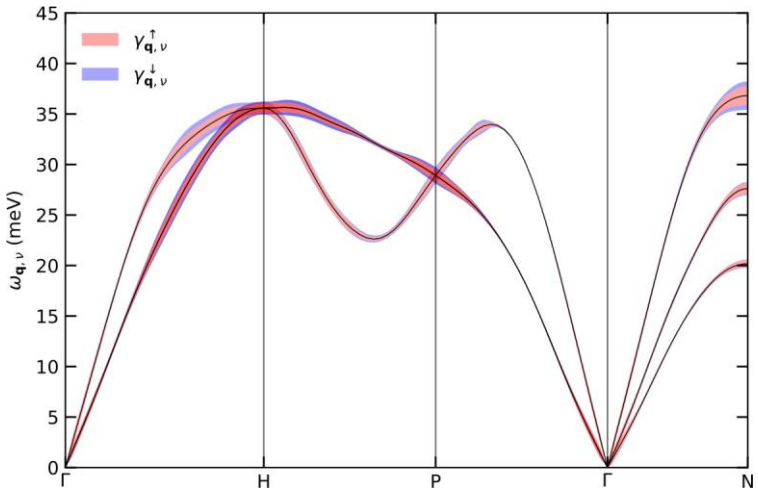

Fig. 2: Spin resolved phonon linewidth in Fe.

ACKNOWLEDGMENTS
We acknowledge support from the project Produrre Idrogeno in Trentino - H2@TN (PAT-Trento)

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EFFECTIVE SINGLE PARTICLE PICTURE FOR ANHARMONIC LATTICE DYNAMICS: A ROSETTA STONE FOR ELECTRONIC AND IONIC RESPONSE

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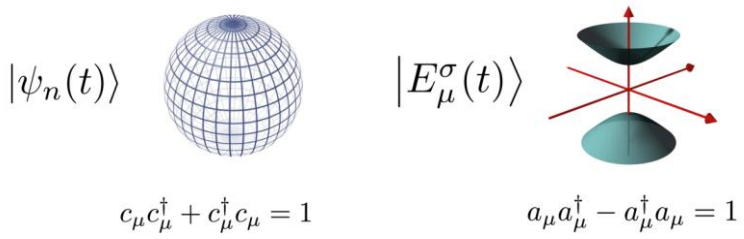
We establish a theoretical framework for the description of the dynamics of a lattice of ions in a mean-field approach, where anharmonicity is included via self-consistency. In this picture, the many-body dynamics of a system of N atoms in 3 dimensions can be mapped in the dynamics of two 6N vectors: the phonon condensate, describing the evolution of the average positions atoms, and the phonon spinors, describing the evolution of the elastic constants of the atoms. The phonon spinors are classified by a quantum number that behaves as a spin: the phonon pseudospin. The many-body Liouville equation is replaced by two wave equations equivalent to the time-dependent Schrödinger equation for the evolution of the electronic wave function in density functional theory. Exploiting this parallelism, we formulate the response of the anharmonic lattice in one-to-one correspondence to the established time-dependent density functional theory for electrons. In complete analogy with the electronic case, we express the ionic response in terms of matrix elements of operators representing external fields and forces. We show how

anharmonicity acts as a phonon screening of the external perturbations, behaving as the Hartree-exchange correlation kernel in electronic theories. By approximating the density matrix as a Gaussian, we recover the equations of the time-dependent self-consistent harmonic approximation. In this case, the linear response equations are formulated in terms of an anharmonic kernel including three- and four-phonon scattering.

Translating the problem of anharmonic lattice dynamics into the language of density functional theory, this work elucidates how the theoretical and computational advances in modeling the dynamical response of interacting electrons can be directly applied to the response of interacting ions. We show how our formalism can be used to devise first-principles calculations of Fano profiles in IR signals of insulators originating from anharmonic screening of optical response associated with anharmonic Born effective charges.



SWITCHABLE CHERN NUMBER IN VAN DER WAALS HETEROSTRUCTURES

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Despite the huge expansion in the family of 2D materials, Chern insulators remain rare, with most monolayers being topologically trivial. However, stacking such trivial materials into van der Waals heterostructures offers vast opportunities for emergent topological phases. Here we show how to engineer topological heterostructures from trivial layers and control their Chern number via an external magnetic field. The key is combining ferromagnetic monolayers–whose valence band edge depends on magnetization direction–with trivial semiconductors having suitable band alignment. This can induce a band inversion–and a topological transition–for one magnetization orientation but not the other, enabling field-tunable topological order. The theoretical scenario is validated through accurate first-principles simulations by screening 2D databases for realistic materials platforms.

ACKNOWLEDGMENTS
We acknowledge financial support from the EMPEROR project, CUP E93C24001040001, funded by the European Union – NextGeneration EU (M4C2INV1.3) through the National Quantum Science and Technology Institute (Spoke 5).

EFFECTS OF EXCITON-PHONON COUPLING ON OPTICAL PROPERTIES OF $MOSE_2$ VIA A CUMULANT APPROACH

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In the last two decades, two-dimensional materials have drawn much interest due to their electrical and optical properties, the latter being dominated by *excitons*. In the Many-Body Perturbation Theory state of the art, excitonic effects are included in absorption spectra by means of the Bethe-Salpeter equation, solved within the static approximation (SBSE) [1, 2]. However, the SBSE fails for those systems wherein the coupling of excitons with other neutral excitations (such as phonons) is non-negligible, since it causes a considerable spectral weight redistribution, with the appearance of additional features called *satellites*.

Going beyond the static approximation and solving the full dynamical BSE with a first-order kernel in the screened interaction would yield spectra with satellites, but unfortunately - besides its extreme complexity - their positions would not be correctly reproduced. Instead, a cumulant approach [3, 4] for the charge response function appears more promising, mapping the problem to that of a particle coupled to bosons.

In the case of the coupling of excitons with phonons [5], it was recently shown [6, 7] how exciton-phonon satellites can be included in the spectra through a cumulant expansion of the two-point polarizability in terms of an effective exciton self-energy, which is evaluated as post-processing of state-of-the-art *ab-initio* calculations. In this poster, I will present the aforementioned procedure and some interesting results coming from its application to the transition metal dichalcogenide monolayer $MoSe_2$, thus explaining how exciton-phonon coupling affects its absorption spectrum.

ACKNOWLEDGMENTS
We acknowledge ISCRA for awarding this project access to the LEONARDO supercomputer, owned by the EuroHPC Joint Undertaking, hosted by CINECA (Italy).

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F-SUM RULE IN BETHE-SALPETER, (SCREENED) HARTREE-FOCK, HYBRID-DFT APPROACHES

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Electrical transport properties in two-dimensional materials are of great interest for their technological applications. As the reduced dimensionality does not allow for sufficient screening of the electron-electron long-range interaction, its explicit treatment, e.g. via the inclusion of the non-local exchange operator, is required. The Bethe-Salpeter equation (BSE), screened Hartree-Fock (TD-sHF) and/or Density-Functional-Theory with Hybrid functionals (DFT-Hybrid) are the main approaches with the desired features, able to take into account also the excitonic effects and suitable for evaluating optical conductivity within linear response theory [1,2]. Within this framework, the f-sum rule plays a pivotal role in validating the consistency of these theories; as an exact quantum-mechanical relation, it provides a fundamental and rigorous constraint on the integrated optical conductivity. While the impact of non-local exchange interaction on the f-sum rule has been investigated in molecular systems [3,4,5], its extension to solid-state materials, particularly metallic ones, where the optical conductivity is characterized by also the additional Drude peak, remains less explored. In this work, we study how the non-local exchange interaction could modify the f-sum rule and redistribute spectral weight between the Drude peak and inter-band transitions. By applying this framework to low-doped graphene, we clarify through a tight-binding model how the non-local exchange interaction shapes electrical transport properties in two-dimensional materials.

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FROM MINIMUM-ENERGY PATHS TO FINITE-TEMPERATURE DIFFUSION: NEB AND ML-ACCELERATED DYNAMICS IN LI_2S

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Activated processes in periodic materials are often governed by rare events whose elementary mechanisms can be characterized through minimum-energy paths, but whose impact on

macroscopic transport requires finite-temperature dynamical sampling. This connection is particularly challenging at the first-principles level, where accurate electronic-structure methods can provide reliable barriers and transition state structures, but direct ab initio molecular dynamics is usually limited to short time and length scales. In this work, we combine first-principles reaction-path calculations and machine-learning-accelerated molecular dynamics to investigate lithium diffusion in crystalline Li_2S. The minimum-energy path calculations are based on the Nudged Elastic Band method recently implemented in the periodic electronic-structure CRYSTAL code. The implementation includes standard NEB together with improved variants such as climbing-image and variable-spring formulations, enabling the study of activated processes in both molecular and periodic systems. Thanks to the use of localized Gaussian basis sets in CRYSTAL, the approach is particularly suitable for performing reaction path calculations even at the hybrid functional DFT level. As a materials application, we focus on lithium migration in Li_2S, a system relevant to solid-state lithium battery interfaces and sulfur-based battery technologies. Candidate migration pathways are first identified through a topological analysis of the electron density, which highlights low-density regions such as ring and cage critical points as possible channels or interstitial sites for Li motion. These pathways are then refined through climbing-image NEB calculations to determine activation barriers and characterize the corresponding transition states. The results show that purely interstitial diffusion is strongly disfavored, whereas mechanisms involving vacancies and Frenkel-type defects are significantly more accessible. In particular, concerted vacancy–interstitial mechanisms lead to the lowest barriers, indicating that defect cooperation can strongly facilitate Li migration in the crystalline phase.

Static pathway calculations, however, do not directly describe the finite-temperature evolution of the system. To bridge this gap, ab initio molecular dynamics simulations are used to assess the activation of the proposed mechanisms at high temperature. Building on these first-principles data, we are extending the sampling through machine-learning interatomic potentials. MACE models trained on PBE0 data using an active-learning strategy, together with DeepMD models for larger pristine Li_2S supercells, are being used to access longer trajectories and larger system sizes. The resulting simulations will allow us to extract descriptors of Li transport. Overall, this combined NEB–BOMD–MLIP strategy provides a route to connect quantum-level minimum-energy path calculations with realistic finite-temperature simulations of ion transport in periodic materials.

ACKNOWLEDGMENTS
This project has received funding from the European Research Council under the European Union's Horizon 2020 research and innovation programme, grant agreement No. 865657, QUANTUMGRAIN. The authors acknowledge support from Project CH4.0 under the MUR programme "Dipartimenti di Eccellenza 2023–2027" at the University of Torino. The Atomistic Simulations group at the Istituto Italiano di Tecnologia is also acknowledged for support and discussions.

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SECONDARY ELECTRON EMISSION IN MULTILAYER SYSTEMS

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Università degli Studi Dell'Aquila

The emission of low-energy electrons induced by the impact of energetic primary electrons on a material surface is known as secondary electron emission (SEE). It is a fundamental process governing electron–matter interactions. The resulting secondary electron yield (SEY), defined as the ratio between emitted secondary electrons and incident primary electrons, plays an important role in numerous applications, such as particle accelerators, detectors, and space technologies. Accurate prediction of SEY requires a detailed description of electron transport, inelastic scattering processes, and the dielectric response of materials.

In this work, a Monte Carlo framework for the simulation of secondary electron emission is developed and extended to the treatment of multilayer systems. Material dependent quantities, including the Fermi level and momentum-dependent energy loss function, are obtained from first-principles calculations based on density functional theory using ab-initio codes. The implementation is validated against established Monte Carlo SEE simulations for bulk aluminum and copper and is subsequently applied to Cu/Al and Al/Cu multilayer systems with varying coating thicknesses.

The results demonstrate a strong dependence of the secondary electron yield on both coating thickness and stacking order. While the Cu/Al configuration follows analytical thickness dependent models commonly used in the interpretation of experimental measurements, the Al/Cu system exhibits qualitatively different behavior, showing the limitations of simplified analytical descriptions for asymmetric multilayer systems. These results highlight the importance of explicitly modeling electron transport across material interfaces and establish the proposed approach as a flexible framework for the investigation of secondary electron emission in complex layered materials.

TDDFT FORCES REVEAL THE LIMITS OF ΔSCF FOR DIAMOND DEFECTS

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Defects in semiconductors are promising candidates for solid-state qubits because their

energy levels can be well isolated from the environment. Accurately predicting their optical properties is therefore essential for discovering new quantum systems [1]. Constrained-occupation Density Functional Theory (ΔSCF) is widely used to calculate excited-state properties, including zero-phonon lines (ZPLs), due to its low computational cost. However, its reliability is not always guaranteed. Here, we benchmark ΔSCF against time-dependent density functional theory (TDDFT) for a diverse set of diamond defects from the ADAQ database [2,3]. Excited-state geometries are optimized using analytical nuclear gradients implemented in the WEST code [4–6]. We find that ΔSCF can produce large ZPL errors when defect states strongly hybridize with the bulk bands of diamond. Our results identify when ΔSCF remains reliable and when more accurate TDDFT calculations are required, providing practical guidelines for the computational discovery of solid-state qubits.

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LONG-RANGE ELECTROSTATICS IN ATOMISTIC MACHINE LEARNING: A PHYSICAL PERSPECTIVE

Federico Grasselli

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The inclusion of long-range electrostatics in atomistic machine-learning models is attracting increasing attention as a route toward quantum-mechanical accuracy in the prediction of molecular and materials properties. Despite this progress, a general prescription is still lacking for how long-range physical effects should be incorporated while preserving the locality principles that underlie most transferable machine-learning representations.

This contribution provides a physical perspective on this problem by discussing how different electrostatic contributions can be represented through distinct learning paradigms. We distinguish between local charge models, based either on explicit charge-density decompositions or on implicit auxiliary variables, and approaches in which nonlocality is deliberately introduced, for example through self-consistent procedures, nonlocal descriptors, or nonlocal learning architectures. We also discuss the related problem of finite-field effects, where the coupling to the system polarization becomes essential for describing the response to an external electric bias, and we examine the implications of different modeling choices for simulations of electrochemical interfaces and ionic transport.

ACKNOWLEDGMENTS
This work is based upon activities from COST Action CA22154 – Data-driven applications towards the engineering of functional materials: an open network (DAEMON), supported by COST (European Cooperation in Science and Technology).

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MULTIPOLAR ORDER IN DOUBLE PERVOSKITES OSMATES: A NMR AND MUSR INVESTIGATION

Anshu Kataria[1], Dario Fiore Mosca[2], lija K. Nikolov[3], Giuseppe Allodi[1], Patrick M. Woodward[4], Vesna F. Mitrovic[3,5], Cesare Franchini[2,6], Samuele Sanna[6] and Pietro Bonfa[7,8]

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Here, we investigate the 5d2 double-perovskite osmates Ba2CaOsO6, which provide a unique provide a unique platform to study the unconventional ordered states, where the interplay between spin, orbital, charge, and lattice degrees of freedom is at play [1–4]. In particular, in Ba2MOsO6 (where M is the diamagnetic ion), the electronic occupation of the Os 5d orbitals (depending on M ion) has been suggested to host quadrupolar ordered as well as multipolar ground states associated with strong spin-orbit coupling and coupling between electronic and lattice degrees of freedom [5–7]. However, without the conventional magnetic dipolar order, these states are extremely difficult to detect using standard measurement techniques. Thus, we employ complementary local-probe techniques, including nuclear magnetic resonance (NMR) and muon spin relaxation and rotation (μSR), which are highly sensitive to subtle changes in the local electronic and magnetic environment. We combine experimental results with density functional theory calculations to present a unified microscopic picture of the multipolar ground state. The combined approach corroborates the proposed multipolar-order scenario and provides a consistent interpretation of previous observations and theoretical results.

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Session 2 – Thursday the 27th of August 2026 – 17:30-19:00

Kaushik Vansh	A Multiscale Framework for Accurate Electron Transfer in Organic Systems
Kortstee Alex	Machine-Learning Force Fields for Predicting the Raman Spectrum of KTaO3
Leoni Luca	Machine-learned dynamics of surface polarons at reduced oxide surfaces
Macheda Francesco	Electronic transport in BN-encasulated graphene limited by remote phonon scattering
Mamlouk Mohamed	Intelligent Molecular Switches for Brain-like DevicesMarques Miguel - Ruhr Universitaet Bochum - Machine Learning-Accelerated Discovery of High-Temperature Superconductors
Mitoli Davide	Anharmonic Vibrational Spectra of Solids from First-Principles with CRYSTAL
Pecorella Francesco	Thermal and Non-Thermal Melting of Germanium
Pintus Andrea	Dynamic Scham Schluter equations
Settembri Paolo	Capturing Nuclear Quantum Effects in High-Pressure Superconducting Hydrides and Ice with Nuclear–Electronic Orbital Theory
Sharma Preeti	Electronic invesigation of reconstructed polar CuI(111) surface
Sun Dewen	Exploring High Entropy Oxide Structures with Machine Learning Interatomic Potentials: Direct Comparison of Molecular Dynamic Simulations with Experimental Observations
Varrassi Lorenzo	High-throughput workflows and machine-learning models for GW quasiparticle corrections
Volpato Giulio	Density functional theory for superconductors in a Wannier functions framework
Zhu Xiangzhou	Light-Induced Ultrafast Control of Polarization and Magnetization in Semiconductors
Zuccolin Walter	Ab-Initio Comparison of Semiconductor and Insulator Monolayers on Metal Surfaces: hBP vs hBN

A MULTISCALE FRAMEWORK FOR ACCURATE ELECTRON TRANSFER IN ORGANIC SYSTEMS VIA CONSTRAINED DFT AND CLASSICAL MOLECULAR DYNAMICS

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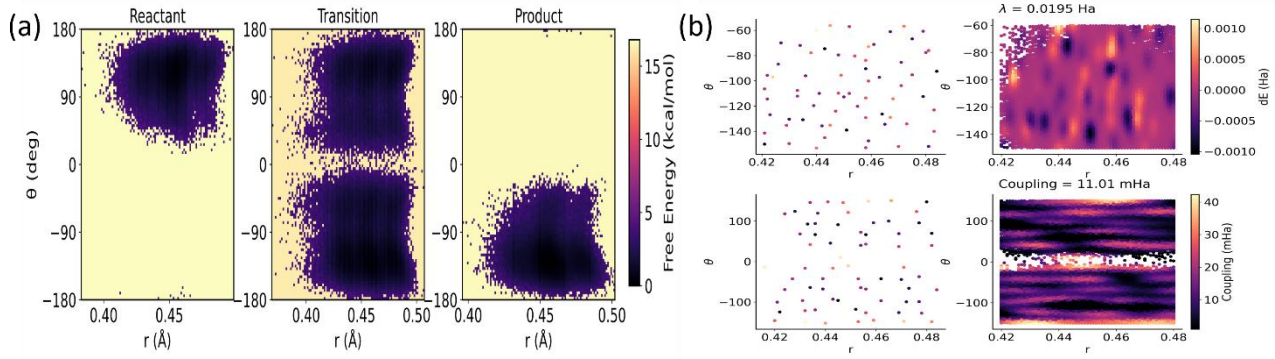
Accurate prediction of electron transfer in organic systems requires reliable evaluation of reorganization energy and electronic couplings while explicitly accounting for solvent effects. Standard vacuum quantum mechanical approaches often deviate from experimental observations due to the absence of environmental fluctuations, whereas fully *ab initio* molecular dynamics is computationally too expensive for realistic systems.

We present a multiscale framework combining classical molecular dynamics (MD), constrained density functional theory (CDFT), and kernel regression to model electron transfer in organic mixed-valence systems. Classical MD is used to sample thermally accessible solvent configurations, capturing both donor–acceptor distance and relative molecular orientation. Selected

configurations are evaluated using CDFT to compute electronic couplings and vertical energy gaps, which define the electron transfer reaction coordinate. Kernel regression is then used to interpolate these quantities across configurational space, enabling efficient reconstruction of free-energy surfaces and extraction of reorganization energies and couplings.

This approach provides a computationally efficient and physically grounded alternative to fully *ab initio* simulations and enables future development of machine learning models for predictive electron transfer in complex molecular environments.



Fig(a): Classical molecular dynamics sampling of solvated electron transfer configurations in distance–orientation space. Fig (b) : Kernel regression reconstruction of electron transfer properties from CDFT data, yielding Coupling and reorganization energy.

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MACHINE-LEARNING FORCE FIELDS FOR PREDICTING THE RAMAN SPECTRUM OF KTAO3

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University of Vienna

Polar ionic compounds, like KTaO3, often display a surface charge density that can be approximated as a two-dimensional electron gas. Recently, however, it was found that this charge density for KTaO3 can be better described by charge density waves, possibly mediated through polarons and bipolarons. If these polarons are present, they would influence the vibrational properties of the surface, which would therefore yield a different surface Raman spectrum. A first step towards identifying such a difference is to establish a reliable method for computing the Raman spectrum of bulk KTaO3.

MACHINE-LEARNED DYNAMICS OF SURFACE POLARONS AT REDUCED OXIDE SURFACES

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Reducible oxides exhibit a rich interplay of electronic, structural, and chemical properties that underpins applications in catalysis, photovoltaics, batteries, and energy storage [1]. This interplay is strongly shaped by excess electrons, often introduced by oxygen vacancies, that localize as small polarons and influence charge transport and surface chemistry [2]. At surfaces, these polarons play a central role in charge localization, mobility, and reactivity, yet their finite-temperature dynamics remain difficult to access from first principles due to the long time scales needed to adequately sample polaron's hopping. To overcome this limitation, we extend machine-learning-assisted polaron dynamics [3] to redox-active oxide surfaces, using oxygen-deficient rutile TiO2(110) as a paradigmatic case. By accessing several nanoseconds of dynamics over a range of temperatures, we show that small-polaron mobility at the reduced rutile TiO2(110) surface is suppressed by several orders of magnitude relative to the corresponding bulk material, providing a microscopic interpretation of the lower electron mobilities observed in porous rutile TiO2 compared with single-crystal samples [4,5,6]. This suppressed mobility arises from the loss of favourable hopping pathways: surface polaron motion is largely confined to planar inter-row trajectories within the second topmost layers, with only rare interlayer hopping events. These results establish a transferable machine-learning strategy for investigating polaron dynamics in reducible oxides.

ACKNOWLEDGMENTS
The authors acknowledge support by the National Recovery and Resilience Plan (NRRP), Mission 4 Component 2 Investment 1.3 - Project NEST (Network 4 Energy Sustainable Transition) and CN-HPC grant no. (CUP) J33C22001170001, SPOKE 7, of Ministero dell'Università e della Ricerca (MUR), funded by the European Union NextGenerationEU. This research was partially funded by the Austrian Science Fund (FWF) 10.55776/F8100 project TACO.

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ELECTRONIC TRANSPORT IN BN-ENCASULATED GRAPHENE LIMITED BY REMOTE PHONON SCATTERING

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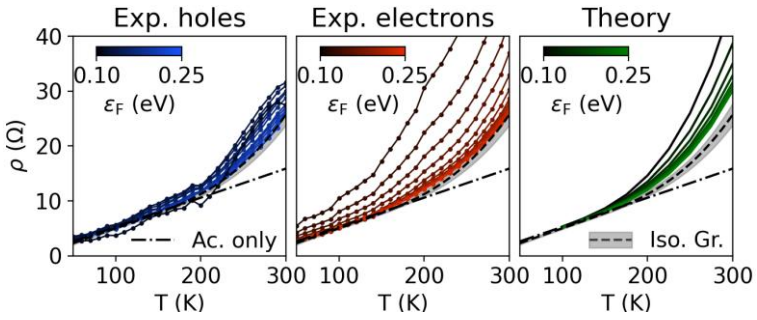
Graphene is renowned for its exceptional electrical properties, but in practical applications it must be protected from environmental degradation. Typically, this is achieved by "encapsulating" graphene between layers of protective materials, usually hexagonal boron nitride (hBN). This encapsulation successfully yields extremely clean, high-mobility devices by shielding the graphene sheet from impurities and extrinsic defects. However, a crucial question remains: does the protective environment itself alter graphene's intrinsic performance? I will present recent experimental [1] and theoretical [1,2] results demonstrating that the encapsulating hBN layers are not entirely passive. Instead, atomic vibrations living in the encapsulator remotely interact with graphene's electrons, significantly increasing the electrical resistivity of graphene up to room temperature. Ultimately, these findings reveal that the encapsulating hBN layers themselves establish a fundamental limit to electronic transport in graphene.



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INTELLIGENT MOLECULAR SWITCHES FOR BRAIN-LIKE DEVICES

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Centre de Nanosciences et de Nanotechnologies (C2N – UMR 9001 CNRS / Université Paris-Saclay)

Brain-inspired computing represents a paradigm shift toward low-power and adaptive information processing by mimicking the dynamic operation of biological synapses, where ionic fluxes and voltage-dependent neurotransmission regulate signal propagation (Figure 1). Emulating such

complex behavior at the molecular scale has become feasible through dynamic molecular switches, which couple charge transport with redox and structural reconfiguration processes [1].

In artificial molecular synapses, signal modulation arises from voltage-driven protonation/deprotonation and redox processes, analogous to the ionic fluxes that govern neurotransmission in biological systems. This coupling between charge transport and chemical reactivity produces hysteretic current–voltage characteristics and negative differential resistance (NDR), providing an electronic analogue of synaptic plasticity [1]. In this study, we investigate how different ionic species **(H^+, Na^+, K^+, etc.)** modulate the electronic response of Au/HNC–quinone/EGaIn molecular junctions. Proton-coupled electron transfer (PCET) at the quinone redox core drives the reversible switching between the fully oxidized (n = 4) and fully reduced (n = 0) states (Figure 2a): sequential protonation of the four carbonyl oxygens converts the quinone into its hydroquinone-like form, while the accompanying electron transfer preserves local charge neutrality.

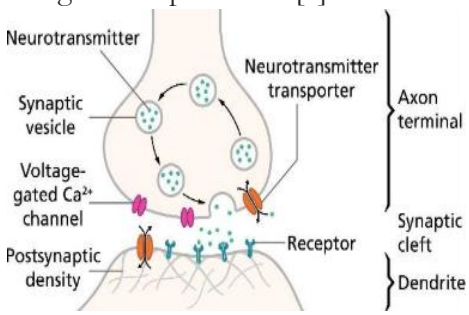

Figure 1. *Schematic of neurotransmitter release and reuptake at a biological synapse, illustrating the ion-mediated signal propagation that inspires ionic control of molecular junctions.*

This redox-driven protonation reorganizes the frontier molecular orbitals of the quinone core: the level that lies as HOMO−1 in the oxidized (n = 4) state rises in energy upon reduction and becomes the new HOMO, shifting closer to the electrode Fermi level. This HOMO−1 → HOMO crossover brings the molecular level into near-resonance with the electrode Fermi level over a narrow bias window, transiently enhancing the tunneling current before it moves out of resonance again. The microscopic origin of the NDR feature. Because the forward and reverse voltage sweeps encounter this level crossing at different biases, the junction displays a pronounced hysteresis loop (Figure 2b), reinforcing the overall memory behavior and paving the way for brain-like molecular devices [2].

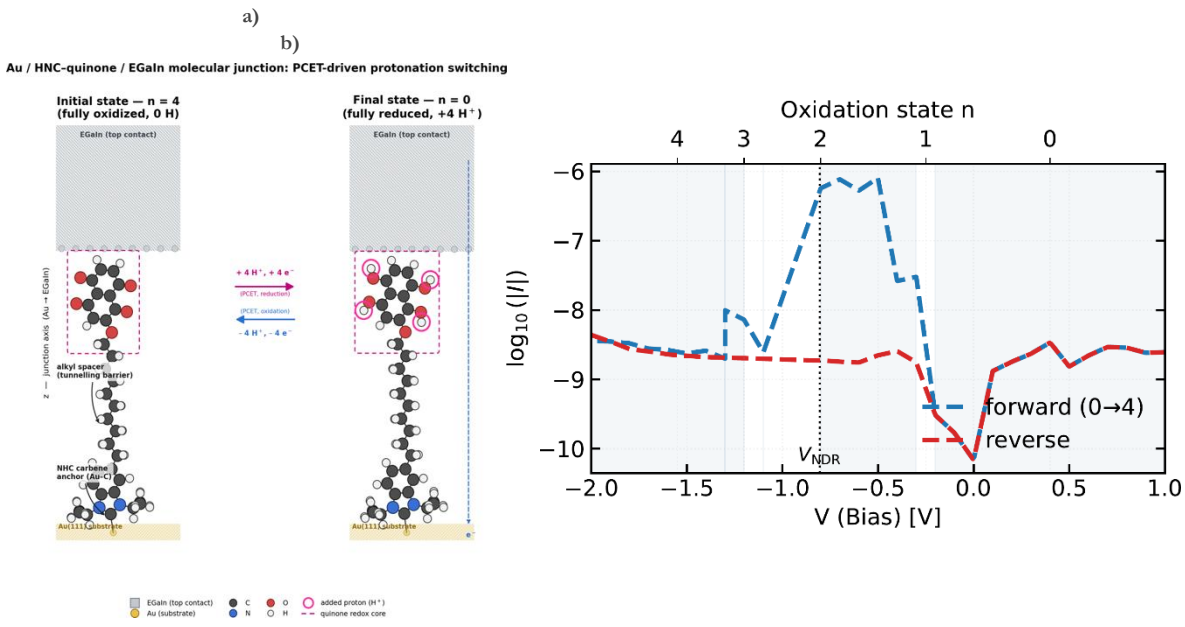

Figure 2. *(a) DFT-relaxed Au(111)/HNC–quinone/EGaIn junction in the initial (n = 4, fully oxidized) and final (n = 0, fully reduced) states. The reversible 4× PCET step ($H^+ + e^-$) protonates the quinone redox core and drives the switching. (b)*

Hysteretic current–voltage response of the junction as a function of the protonation state (oxidation state n = 0–4), showing the emergence of NDR upon forward voltage sweep.

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ANHARMONIC VIBRATIONAL SPECTRA OF SOLIDS FROM FIRST PRINCIPLES WITH CRYSTAL

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The accurate description of anharmonic vibrational properties of solids still represents one of the greatest challenges in modern theoretical chemistry and condensed-matter physics. In this contribution the theoretical and computational framework for the anharmonic description of vibrational spectroscopies in the CRYSTAL code is presented.

Evaluation of quadratic, cubic and quartic terms of the potential is performed through numerical differentiation [1]. Anharmonic vibrational states can be computed at different levels of approximation, ranging from a single-mode anharmonic oscillator approach, in which phonon-phonon couplings are neglected, to more sophisticated methods such as Vibrational Self-Consistent Field (VSCF) and Vibrational Configuration Interaction (VCI) [2]. While VSCF accounts for phonon–phonon interactions within a mean-field framework, VCI provides a more explicit treatment of vibrational couplings, albeit at a substantially higher computational cost. To reduce the associated memory and time requirements, a Subspace Iterative VCI (SI-VCI) scheme has been implemented, improving the efficiency of conventional VCI calculations [3]. Infrared (IR) and Raman intensities are subsequently evaluated from transition moments between the initial and final anharmonic vibrational states obtained with the approaches [4, 5]. These methodologies have been successfully tested and applied to dry ice and thiourea, two molecular crystals exhibiting strong anharmonic features in their IR and Raman spectra.

ACKNOWLEDGMENTS
This research has received funding from the Project CH4.0 under the MUR program "Dipartimenti di Eccellenza 2023-2027" (CUP: D13C22003520001).

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THERMAL AND NON-THERMAL MELTING OF GERMANIUM TELLURIDE

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Phase-change materials (PCMs) are compounds that exhibit significant differences in electrical resistivity and optical properties between their crystalline and amorphous phases. These characteristics, combined with a fast crystallization rate, make them highly suitable for applications such as non-volatile memory devices, where short laser pulses are used to induce order–disorder phase transitions to write and erase information [1].

A notable example of a PCM is Germanium Telluride (GeTe), which exhibits a crystalline rhombohedral phase at ambient temperature [2] and a rock-salt cubic structure above 700 K [3-4]. Applying femtosecond visible laser pulses induces a non-thermal transformation from the rhombohedral to a mixtures of cubic and rhombohedral phase [5,6] at intermediate fluences (20mJcm-2, ref. [5]). Furthermore, when the laser fluence exceeds a certain threshold (>30mJcm-2, ref. [5-7]), the sample can undergo amorphization [5-7]. Static ab initio studies have shown that these non-thermal effects driving the rhombohedral-to-cubic transition differ from the thermal one [6]. However, whether the non-thermal pathway leading to the liquid state and then to the amorphous state is the same as the conventional thermal melting process remains still unknown.

In this work, we address this open question by directly investigating the non-thermal pathway leading to the liquid phase in GeTe. To systematically compare the thermal and non-thermal liquid states, we first trained and validated a MACE [8] machine-learning interatomic potential for the rhombohedral, cubic, and liquid phases. Furthermore, in order to capture the effect of the fs pulse and the consequent non-thermal process, we train a MACE potential on a set of excited crystalline configurations generated via the constrained density functional perturbation theory (cDFPT) approach explicitly including electron-hole plasma effects [9]. We then simulate and compare the mechanisms of thermal and non-thermal melting, outlining the similarities and key differences between the two processes.

ACKNOWLEDGMENTS
We acknowledge ISCRA for awarding this project access to the LEONARDO supercomputer, owned by the EuroHPC Joint Undertaking, hosted by CINECA (Italy).
This study has been funded by PRIN 2022– NextGenerationEU, "Non-equilibrium routes to control the switching cycle in phase-change materials" - 2022KT8MM3 - CUP E63C22000860006 and by the European Union (ERC, DELIGHT, 101052708).

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SOLVING THE DYNAMICAL SHAM-SCHLÜTER EQUATION USING THE SUM-OVER-POLES FORMALISM

Andrea Pintus, Andrea Ferretti and Nicola Marzari

EPFL

Kohn–Sham density-functional theory (DFT) provides an efficient framework for calculating the ground-state electronic properties of molecules and materials by mapping the interacting many-electron problem onto an auxiliary non-interacting system. However, its static and local exchange-correlation potential does not directly provide the spectral information required to describe charged excitations and photoemission spectra. Such properties are commonly addressed using many-body perturbation theory, where the electronic structure is described through a non-local and frequency-dependent self-energy. An alternative route consists in mapping the many-body self-energy onto a local but frequency-dependent spectral potential [1]. This potential can, in principle, be determined through a dynamical generalization of the Sham–Schlüter equation [2,3], such that the auxiliary system reproduces the spectral density of the interacting Green's function. Despite its appealing connection between many-body perturbation theory and an effective single-particle description, the practical solution of the resulting frequency-dependent integral equation remains challenging.

In this work, we propose a strategy to solve the dynamical Sham–Schlüter equation using the Sum-over-Poles formalism [4,5]. Green's functions, self-energies, and dynamical potentials are represented in terms of their poles and matrix-valued residues. This representation permits products, inversions, and Dyson equations to be treated directly in frequency space, replacing numerical frequency convolutions and integrations with algebraic operations among pole expansions. We apply the approach to the full dynamical Sham–Schlüter equation and investigate

the construction of a local, frequency-dependent potential from a given many-body self-energy. The resulting framework provides a practical route for evaluating spectral potentials and constitutes a step toward the numerical implementation of density-functional theories based on the spectral density.

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CAPTURING NUCLEAR QUANTUM EFFECTS IN HIGH-PRESSURE SUPERCONDUCTING HYDRIDES AND ICE WITH NUCLEAR–ELECTRONIC ORBITAL THEORY

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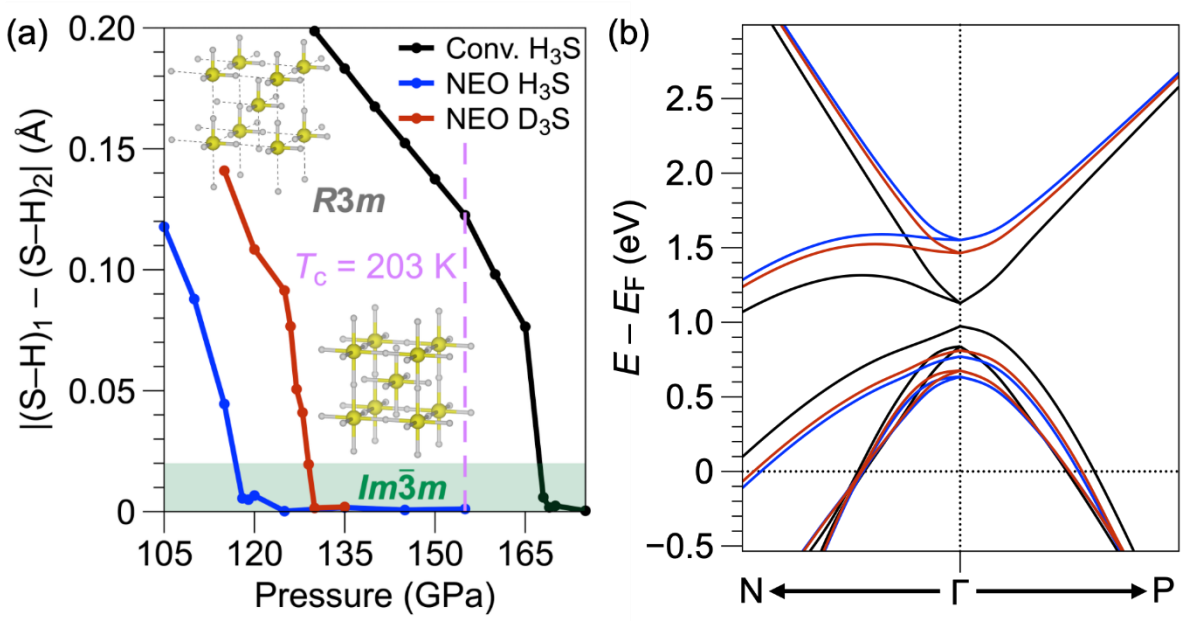
Nuclear quantum effects are essential for correctly describing hydrogen-rich materials at high pressures. Superconducting hydrides and ice are prime examples of such systems, requiring the inclusion of lattice anharmonicity and nuclear quantum effects to correctly predict and describe the structures and phase transition pressures observed experimentally. Herein, we show that the nuclear–electronic orbital density functional theory (NEO-DFT) method, which treats specified nuclei quantum mechanically on the same level as the electrons, is capable of accurately describing nuclear quantum effects in superconducting hydrides and ice. NEO-DFT predicts the hydrogen-bond symmetrization pressure in H_3S and D_3S, benchmarking against the more expensive stochastic self-consistent harmonic approximation method, and predicts the correct symmetric $Fm\bar{3}m$ structure for LaH_{10} at a wide range of pressures. NEO-DFT also predicts the ice VIII to ice X phase transition pressures for H_2O and D_2O in agreement with experimental measurements. The accuracy, computational efficiency, and broad applicability of the NEO method opens the door for expanded large-scale studies into these types of systems. (1)



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RECONSTRUCTION-DRIVEN ELECTRONIC LANDSCAPES OF POLAR CUI(111) SURFACE

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Copper iodide (CuI) is a promising p-type transparent semiconductor for optoelectronic pplications, yet the atomic and electronic structure of its polar (111) surface remains poorly understood. Using density functional theory cal-culations, we systematically investigate both Cu-terminated and I-terminated CuI (111) surfaces, analyzing various reconstruction models including vacancy-buckling and trimer configurations. Our structural analysis reveals that Cu-terminated surfaces with Cu vacancies and I-terminated surfaces with I va-cancies exhibit nearly identical low surface energies (about 5.6-5.7 meV/A˚2), indicating comparable thermodynamic stability through effective polarity com-pensation. The Cu-vacancy reconstruction on Cu-terminated surfaces exhibitsp-type semiconducting behavior, making it suitable for hole transport applica-tions, while the I-vacancy reconstruction on I-terminated surfaces shows n-type character with disperse in-gap bands. In contrast, I-trimer reconstructions in-troduce localized mid-gap surface states that can act as recombination centers. Our electronic structure calculations demonstrate that surface termination crit-ically influences the work function and charge carrier properties. These findings

provide atomic-level insights into CuI (111) surface stability and electronic char-acteristics, offering guidance for interface engineering in transparent electronics and photovoltaic devices.

EXPLORING HIGH ENTROPY OXIDE STRUCTURES WITH MACHINE LEARNING INTERATOMIC POTENTIALS: DIRECT COMPARISON OF MOLECULAR DYNAMIC SIMULATIONS WITH EXPERIMENTAL OBSERVATIONS

Dewen Sun

Ruhr Universität Bochum

High-entropy oxides (HEOs) is a group of material with complex composition and tunable functional properties, making them attractive for a wide range of energy and electronic applications. However, their structural complexity presents significant challenges for both experimental characterization and ab-initio simulations. The recent emergence of universal machine learning interatomic potentials (uMLIPs), however, has presented a new path for investigating such materials. In this work, we demonstrate that state-of-the-art MLIPs can model the atomic structure and thermodynamic behavior of HEOs with near ab-initio accuracy at experimentally relevant conditions. The structural evolution for CuCoNiZnMgO and CaCoNiZnMgO are computed through molecular dynamic combined with Monte Carlo atom swaps (MDMC). The obersations are directly compared with experimentally synthesized HEO samples showing strong agreements in predicting the phase stability of the systems. This demonstrate that uMLIPs can reliably predict the equilibrium structures of complex materials outside of their training data. This should establish uMLIPs an effective tool for the accelerated design and understanding of high-entropy oxides.

HIGH-THROUGHPUT WORKFLOWS AND MACHINE-LEARNING MODELS FOR GW QUASIPARTICLE CORRECTIONS

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Accurate excited-state electronic properties are essential for the predictive design of electronic, optoelectronic and correlated materials. However, the routine use of GW in high-throughput studies remains challenging because quasiparticle energies depend on a large set of interdependent numerical parameters, and achieving convergence across this multidimensional space is both complex and computationally demanding. As a result, the steep cost of GW calculations still limits their application in large-scale screening studies [1,2]. To address these challenges, we present a fully-automated open-source workflow for G0W0 calculations[3] within the AiiDA framework[4]. The workflow is based on an efficient estimation of the errors due to basis-set truncation and

ultra-soft PAW potentials norm violation, which allows a reduction in the dimensionality of the parameter space and avoids the need for multidimensional convergence searches. To demonstrate the effectiveness of the approach, a database of QP energies for a dataset of over 320 bulk structures is developed in the high-throughput approach. Using this database as a foundation, we then assess machine-learning models aimed at predicting GW quasiparticle corrections directly from DFT-level information. In particular, we investigate the role of state-resolved electronic descriptors [5], alongside structural and compositional descriptors, in learning quasiparticle corrections across the database. Our results show that descriptor-rich models can reproduce GW corrections with useful accuracy, supporting their potential use for accelerated exploratory screening.

DENSITY FUNCTIONAL THEORY FOR SUPERCONDUCTORS IN A WANNIER FUNCTIONS FRAMEWORK

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Density-functional theory for superconductors [1, 2, 3, 4] relies on the solution of a self-consistent equation for the superconducting gap. The kernel of this equation has dominant contributions close to the Fermi surface, hence requiring ultradense k-point sampling.

In the Superconducting-Toolkit (SCTK) code [5] this issue is solved by using an auxiliary energy grid and a reverse interpolation of the density of states. Still, the final nk-resolved gap is limited to coarse k-grids due to the heavy computational cost of ab-initio calculations of the electron-phonon matrix elements.

We overcome this limitation by Wannier interpolating the electron-phonon matrix elements [6, 7, 8], on a set of random points sampled from a distribution peaked at the Fermi surface, and develop a complete Wannier function approach to the solution of SCDFT equations.

ACKNOWLEDGMENTS
Funded by the European Union (ERC, DELIGHT, Grant No. 101052708).

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LIGHT-INDUCED ULTRAFAST CONTROL OF POLARIZATION AND MAGNETIZATION IN SEMICONDUCTORS

Xiangzhou Zhu[1], Stefano Mocatti[1], Junfeng Qiao[2], Nicola Marzari[2], and Matteo Calandra[1]

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Ultrafast optical control of ordered states offers a route toward high-speed functional materials. However, in ferroelectrics optical switching often relies on interlayer sliding or structural distortions, which can limit the speed of polarization control. In magnetism, optical control is commonly associated with angular-momentum transfer mechanisms using circularly polarized light, whereas inducing magnetization with linearly polarized light is consider to be rare. Here, we show that photoexcited carriers provide a route to transiently controlling polarization and magnetization in semiconductors, combining constrained density-functional theory, real-time many-body simulations, and high-throughput first-principles screening.

First, we demonstrate that rhombohedrally stacked transition-metal dichalcogenide bilayers can undergo a transient reversal of their out-of-plane polarization through layer-selective charge redistribution, without interlayer sliding. The reversal develops within a few hundred femtoseconds at moderate carrier densities and is therefore substantially faster than structurally driven switching.

Second, we identify broad class of nonmagnetic semiconductors in which linearly polarized optical excitation can induce exchange-driven spin polarization. Strong responses are favored by narrow transition-metal (d)-derived states near the band edges, while their orbital character and local coordination determine the magnitude and ordering of the induced magnetic moments.

These results establish the spatial and orbital distribution of photoexcited carriers as a unifying design principle for transient control of functional order in semiconductors.

ACKNOWLEDGMENTS
Funded by the European Union (ERC, DELIGHT, 101052708)

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DISTINCTIVE PROPERTIES OF HEXAGONAL BORON PHOSPHIDE WITHIN THE FAMILY OF ATOMICALLY FLAT 2D MATERIALS: AN *AB INITIO* INVESTIGATION

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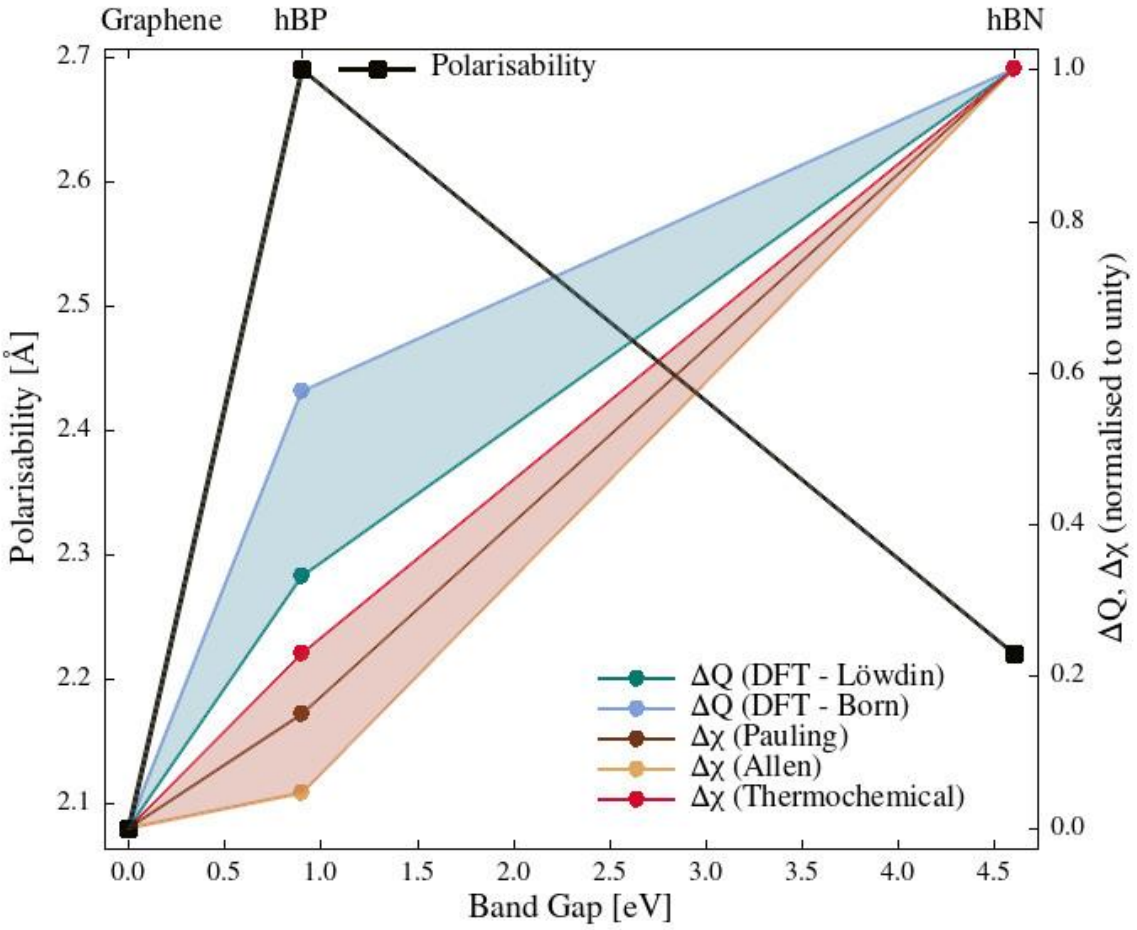
Single-layer hexagonal boron phosphide (hBP) is a predicted honeycomb-structured semiconductor [1] exhibiting interesting properties for photovoltaic and photocatalytic applications [2] filling the void between graphene and hBN and completing the group of atomically flat materials, but its growth remains challenging.

Our previous ab-initio calculations [3] predicted hBP to interact relatively strongly with all the (111)-terminated d-shell metallic substrates commonly employed for epitaxial growth. Au and Ag exhibit the weakest coupling to hBP, making them promising candidates for the exfoliation and transfer of the supported monolayer. In contrast, Pt represents an attractive growth template due to its minimal lattice mismatch with hBP, despite its stronger interaction with the semiconductor. While capping Pt (111) with a single Ag or Au layer reduces the interaction to a level comparable to that of the corresponding bare noble-metal substrates, the residual coupling remains sufficiently strong to suppress the semiconducting character of hBP.

To understand the peculiar properties of hBP, we compare with ab-initio calculations its characteristics with those of graphene and hBN in both free-standing and supported configurations. We found that, while hBN and graphene interact with the respective substrate mainly through weak Van der Waals forces [4], as already reported in literature, hBP displays the characteristic charge density behaviour associated with a covalent-like quasi-bonding [5]. This behaviour can be related to the different intrinsic properties of the three 2D materials. In particular, unlike the bond polarity, quantified though the electronegativity difference $\Delta\chi$ and the computed charge transfer ΔQ between the constituents atoms, which increases from graphene to hBP and hBN, the out-of-plane polarisability follows a different trend, reaching its maximum value in hBP (Figure below).



ACKNOWLEDGMENTS

Authors acknowledge support from the project QUBOP within the PRIN 2022 initiative funded by European Union – Next Generation EU (PNRR Investimento M4.C1, CUP J53D23001410006) through MUR — Italian Ministry for Universities and Research, and from ICSC – Centro Nazionale di Ricerca in High Performance Computing, Big Data and Quantum Computing, funded by European Union – Next Generation EU (PNRR Investimento M4.C2.1.4, CUP J93C22000540006).

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