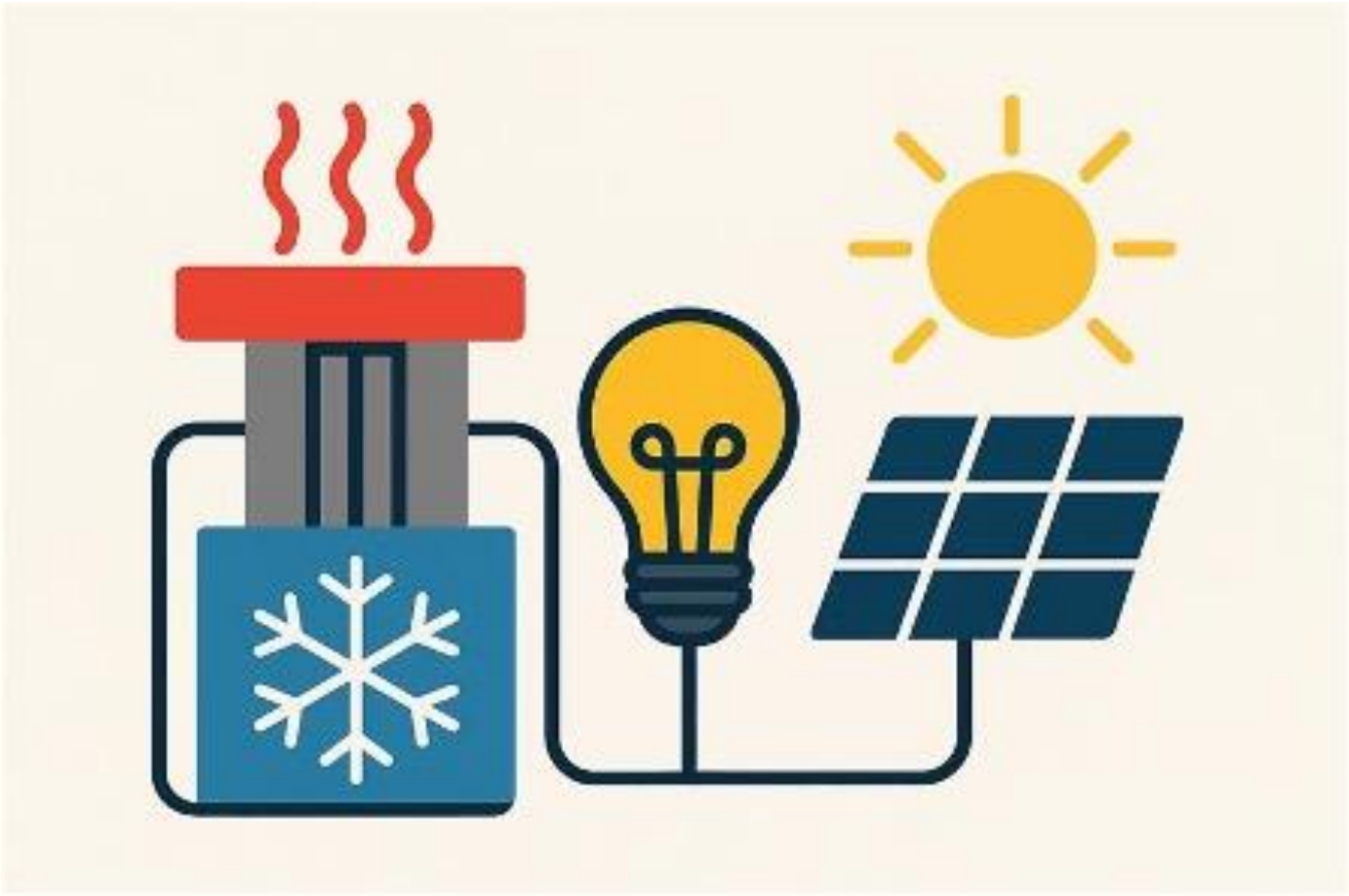

Thomas Young Centre

TYC 8th Energy Workshop: From Electron and Phonon Interactions to Net Zero

1-3 June 2026

Programme & Abstracts

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Day 1 – 1 June 2026

Session 1: Thermoelectric materials I

Current and emerging areas in thermoelectric research

G. Jeffrey Snyder, Northwestern University, Evanston IL, USA [plenary]

Thermoelectrics are often considered for producing electricity from waste heat but actually have much larger application in temperature measurement, solid-state cooling and thermal management. The field of thermoelectrics changed since the proposals to use quantum confinement, electron filtering and nanostructures for phonon scattering. In this talk we will review how this discussion has evolved into a consideration of band degeneracy and grain boundary engineering. While introducing nanoscale interfaces easily lowers lattice thermal conductivity that can now be imaged directly by scanning thermoreflectance, the electrical resistance at grain boundaries has an even greater effect on thermoelectric performance. The detailed understanding of interfaces and microstructure, that not all interfaces and grain boundaries affect thermal and electrical properties the same will usher in a new era of microstructure engineering thermoelectric materials and functional materials in general.

First-Principles and Machine-Learning Exploration of Energy Harvesting Heusler Alloys

Terumasa Tadano, National Institute for Materials Science, Tsukuba, Japan [invited]

Heusler alloys (X_2YZ and XYZ) have been extensively studied as functional materials due to their desirable structural, magnetic, and transport properties. For instance, half-Heusler alloys (XYZ) are known to exhibit low thermal conductivity (κ), which is advantageous for enhancing the *longitudinal* thermoelectric (TE) figure of merit, given by $ZT = S^2\sigma/\kappa$, where S is the Seebeck coefficient and σ is the electrical conductivity. Furthermore, a large anomalous Nernst coefficient (S_{ANE}) has recently been reported for the $L2_1$-ordered Heusler alloy Co_2MnGa [1], demonstrating the potential of magnetic Heusler alloys to achieve high *transverse* TE efficiency, expressed as $Z_{\mathrm{ANE}}T = S_{\mathrm{ANE}}^2\sigma/\kappa$. Given the vast compositional space of Heusler alloys, it is likely that many more functional compositions are yet to be discovered.

To efficiently explore this extensive Heusler space, we conducted systematic first-principles calculations for approximately 27,000 ternary Heusler alloys and evaluated their stability and properties [2]. In addition to conventional stability metrics such as formation energy and hull distance, our study assessed magnetic and phonon stability on an unprecedented scale, enhancing the reliability of our predictions. Moreover, we calculated the lattice thermal conductivity (κ_L) using the Boltzmann transport equation with three-phonon interactions for ~3,000 alloys and the anomalous Nernst conductivity (α_{xy}) using linear response theory for ~5,000 alloys. This high-fidelity data has led to the identification of numerous materials with low κ_L and high $|\alpha_{xy}|$. Some materials exhibit low κ_L and high $|\alpha_{xy}|$ simultaneously, making them particularly attractive for transverse TE applications. In this talk, we will also present machine-learning models [3] trained on the generated data and their applications to exploring vaster quaternary and all-*d* Heusler space.

[1] A. Sakai *et al.*, Nat. Phys. 14, 1119 (2018).
[2] E. Xiao and T. Tadano, Acta Materialia 297, 121312 (2025).
[3] E. Xiao and T. Tadano, npj Comp. Mater. 12, 133 (2026).

Diverse Polymorphism in Chalcogenide Perovskites

Prakriti Kayastha, University College London [contributed]

Chalcogenide perovskites such as BaZrS_3 have gained popularity for their potential in photovoltaic and thermoelectric applications.[1] Synthesis and computational studies of these perovskites have revealed that competing phases, such as the Ruddlesden-Popper (RP) phases.[2,3] These are layered semiconductors with tuneable properties and chemical stability, making them promising candidates for a wide range of functional energy applications. Over the past four decades, the structural diversity of RP oxides has been exploited to realize advanced functionalities; however, similar strategies have not yet been applied to RP chalcogenides, whose structural behaviour remains poorly understood.

In this talk, I will present a bespoke high-accuracy machine-learned interatomic potential that performs large-scale molecular dynamics simulations of the homologous RP series Ba_{n+1} Zr_n S_{3n+1}. We identify new polymorphs for each n value, predict the corresponding phase transition temperatures, and validate our approach through comparison with existing experimental data. We find that the n =1 phase exhibits in-plane negative thermal expansion, and that the n =1 and n =3 phases undergo unusual ascending symmetry breaking, and that phases with n ≥3 develop layer-dependent tilt patterns not previously observed in inorganic RP compounds. This distinctive behaviour arises from the interplay between ZrS6 octahedral rotations and BaS rumpling at the perovskite-rock salt interface, suggesting new strategies for realizing advanced functionalities and tuning properties in RP chalcogenides. Our approach provides new phases in the RP chalcogenide family that must be studied alongside perovskite materials, as the presence of these phases can be integral for tuning the properties of functional materials in thin film technologies.

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[1] Sopiha et al. (2022) Adv Optical Mater.,10(3), 2101704.
[2] Pradhan et al. (2024) Mater. Chem. Frontiers, 8(20), 3358.
[3] Kayastha et al. (2023) Solar RRL, 7(9), 2201078.
[4] Kayastha et al. (2026) Phys. Rev. Lett. 136, 086101.

Session 2: Thermoelectric materials II

From Scattering-Tuned High-Power Metallic Thermoelectrics to Real-World Applications in Waste Heat Recovery

Andrej Pustogow, Institute of Solid-State Physics, TU Wien, 1040 Vienna, Austria [invited]

Thermoelectric (TE) materials directly transform thermal into electrical energy and vice versa, making them promising for a plethora of exciting novel applications. However, state-of-the-art semiconductors did not yet result in broad applications due to low power density and poor mechanical properties. Metallic materials would be superior in this regard but remained largely neglected by the TE community over the past century.

The fundamental research project METHEL (funded by ERC) explores metallic TE via the innovative enhancement principle of tuning electronic interband scattering, that is cardinally different from those applied in semiconductors so far. Here we utilize a synergistic combination of synthesis, spectroscopy, microscopy and high-throughput computational materials screening to realize ultrahigh TE performance in metals. Using this paradigm, we recently discovered record-high power factors (PF) of 34 mWm−1K−2 in binary Ni*x*Au1-*x* alloys, yielding the highest $zT \approx 0.5$ among all metals [1]. Despite this unprecedented TE performance, the high cost of Ni*x*Au1-*x* poses difficulties for applications. We have therefore continued our quest for metallic TE with superior functional properties from more abundant

elements. Utilizing an automated materials screening approach, we discover ultrahigh PF up to 11 mWm−1K−2 near room temperature in the textbook metal Ni3Ge – notably, our theoretically predicted Seebeck coefficient fits experiment perfectly [2]. In our search for novel physical mechanisms to tailor electronic scattering, we identify topological flat bands induced by geometrical frustration as a powerful tool to boost the performance of metallic TE beyond the record-high performance of Ni*x*Au1-*x* [3]. With the novel family of kagome metals $zT > 1$ at room temperature is within reach – exceeding *all* state-of-the-art semiconductor thermoelectrics [3].

To ultimately bring TE materials into real-world applications, the applied project SPIRIT (funded by FFG Austria & EU) utilizes flexible TE generators (FlexTEG from TEGnology in Denmark) for 'green' power generation from waste heat in a biomass thermal power plant (ACCIONA, Spain). This way, TE research in Pustogow Spectroscopy Laboratory truly bridges the gap all way from solid-state theory, materials synthesis and advanced TE measurements to real-world applications. This opens the door for 'game-changer' applications like active cooling – with rapidly growing implementation in microelectronics, optoelectronics, high-power RF devices and bioanalytical platforms – that finally come into reach with the advent of the *Metal Age of Thermoelectricity*.

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[2] Garmroudi, F.; Di Cataldo, S.; Parzer, M.; Coulter, J.; Iwasaki, Y.; Grasser, M.; Stockinger, S.; Pázmán, S.; Witzmann, S.; Riss, A.; Michor, H.; Podloucky, R.; Khmelevskyi, S.; Georges, A.; Held, K.; Mori, T.; Bauer, E.; Pustogow, A., *Sci. Adv.* **11**, eadv7113 (2025). https://doi.org/10.1126/sciadv.adv7113
[3] Garmroudi, F.; Serhiienko, I.; Parzer, M.; Riss, A.; Grasser, M.; Stockinger, S.; Khmelevskyi, S.; Pryga, K.; Wiendlocha, B.; Held, K.; Mori, T.; Bauer, E.; Pustogow, A., *Phys. Rev. X* **15**, 021054 (2025). https://doi.org/10.1103/PhysRevX.15.021054

Advanced Boltzmann transport predictions of thermoelectric effects

Jennifer Coulter, Flatiron Institute, USA [invited]

Accurate computational methods play an important part in understanding the physical origins of high-performing thermoelectric materials. In this talk, I will demonstrate how thermoelectric predictions built on the electron-phonon Boltzmann transport equation can provide insight into experimental results, allowing us to interpret the impressive performance of metallic flat-band materials for potential thermoelectric applications. We find that in these materials, the energy dependence of electron-phonon scattering and beyond-BTE effects are important, highlighting the need for modern computational software taking into account a number of detailed effects.

Anisotropy in phonon and electron transport in Sb2Se3 from machine learning foundation models

Tingwei Li, Imperial College London [contributed]

The comprehensive evaluation of phonon and electron transport has long been hindered by the fundamental trade-off between ab initio accuracy and computational efficiency. The success of machine learning foundation models in mapping potential energy surfaces and electronic Hamiltonian raised the question: can they be extended to predict complex transport properties with high efficiency without sacrificing ab initio accuracy?

To answer this question, in this work, we develop a computational workflow integrating state-of-the-art machine learning interatomic potential MACE-MH-1 and Hamiltonian foundation models Uni-HamGNN to investigate the electron and phonon transport properties in Sb2Se3. The predictive accuracy of this workflow is rigorously validated against semi-density functional theory (semi-DFT)

calculations. Our results reveal both significant phonon and electron transport anisotropy in Sb2Se3: the lattice thermal conductivity exhibits a ~4.1-fold largest anisotropy, reaching ~1.94 W/mK along the ribbon axis (x-axis) and dropping to ~0.65 (y-axis) and ~ 0.47 W/mK (z-axis) across layers. The pronounced anisotropy in phonon transport originates from the spatial distribution of lone-pair electrons. More specifically, the lone-pair electrons are predominantly distributed within the yz-plane, which induces highly asymmetric interatomic forces. This large force asymmetry triggers the highest anharmonic phonon scattering rates, ultimately leading to the ultralow thermal conductivity along the z-direction. Furthermore, the carrier mobilities also exhibit remarkable anisotropy. The electron mobility demonstrates a staggering ~50.1-fold contrast between the x and z directions, while the hole mobility shows a ~4.6-fold variation between the y and z axes. These electronic anisotropies are primarily driven by significant directional variations in electron-phonon coupling strength and carrier effective mass.

This work successfully demonstrates the capability of foundation models to predict complex transport properties with ab initio accuracy and remarkable efficiency in Sb2Se3.

Ab initio thermoelectric transport calculations of alloyed materials

Ankit Kumar, University of Warwick [contributed]

We develop a novel efficient transport method to compute the thermoelectric (TE) power factor (PF) of alloyed materials. We use Boltzmann transport through the ElecTra code [1], which considers the full energy/ momentum dependence of the bands and of the scattering rates using first principles extracted parameters – to date no such method exists for alloys on ab initio basis. The band structure of alloyed materials is computed on a supercell, which results in folded bands, with subsequent band splittings, presenting significant numerical challenges within transport solvers, which we address.

First, we must address the possibility of alloy scattering when alloyed TE is considered. A test case of Si-Ge is presented to show the importance of alloy scattering in the desired range of carrier concentrations. Thereafter calculation of two different alloyed half-Heusler (hH) are carried out using similar calculation approach. First, alloys like Ti1−xZrxNiSn, Zr1−xHfxNiSn, and Hf1−xTixNiSn (x = 0.0, 0.25, 0.50, 0.75, and 1.0) where, we don’t see significant change in the electronic structure (band splitting / broken degeneracy) with x, PF change is observed because of change in band curvature and scattering potentials. Second, TaFeSb type hH, isovalent (Nb) and aliovalent (Ti/Zr/Hf) alloying/doping change the band structure significantly. It was observed that materials with more valley degeneracy are more susceptible to band splitting with alloying and that leads to reduction in the maximum achievable power factor.

These findings are a step forward in understanding the role of alloying on the PF, which would be extremely useful in leading experimental efforts towards high power factor materials.

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Day 2 – 2 June 2026

Session 3: Electron-phonon interactions and energy efficiency

Quantum design of materials for energy-efficient electronics: abstraction, automation, and machine learning

Feliciano Giustino, Austin, Texas [plenary]

The rapid growth of information and communication technology (ICT), driven by data science and artificial intelligence, is placing unprecedented demands on global energy consumption. If current trends persist, ICT could account for a substantial fraction of worldwide electricity use within the next few decades. Addressing this challenge requires a fundamental rethinking of the materials that underpin electronic devices, starting from the transistor.

In this talk, I will discuss how first-principles quantum simulations are enabling the predictive design of materials for energy-efficient electronics. Central to this effort is the ability to compute charge transport properties, such as carrier mobility, by combining density functional theory and many-body perturbation theory with the Boltzmann transport equation. These approaches now achieve quantitative accuracy and allow us to evaluate candidate materials prior to experimental realization.

In particular, I will review recent advances in many-body transport calculations beyond density functional theory, and how the EPW project is evolving to enable exascale computing on GPU accelerators. As illustrative examples, I will present results on strain engineering of wide-bandgap semiconductors and high-throughput searches for high-mobility two-dimensional materials for ultrascaled transistor channels.

Finally, I will introduce emerging computational platforms designed to accelerate materials discovery through abstraction, automation, and integration with modern data-driven approaches. These include the MatCSSI cloud integration, which enables interactive many-body calculations on supercomputers through Jupyter notebooks, and the EPWpy library, which provides high-level abstraction enabling high-throughput and machine learning applications. Together, these developments point toward a future in which quantum simulations, automation, and AI work in concert to design materials for next-generation energy-efficient electronics.

Putting the spin on energy materials: thermoelectric and entropic effects with magnetism

Matthieu Verstraete, University of Utrecht [invited]

A central theme in energy efficiency and edge devices is thermal management: heat evacuation to reduce consumption and heat recovery to power wireless or wearable sensors. Magnetic materials offer specific advantages with additional internal degrees of freedom, whose low energy excitations can be used for information or energy transfer. We will showcase advances in first principles simulations to quantitatively predict (thermo)dynamic and transport coefficients for magnetic solid-state materials, both 2D (CrSBr, CrI3) and 3D (3d FM metals, FeRh). Vibrational and relativistic interactions must be accounted for, and in many cases many-body collective excitations interfere with simple "quasi-particle" representations. We close with an overview of current theoretical methods to capture magnon phonon coupling and a few other routes we are attempting to explore.

X Ma, et al. New Journal of Physics 25, 043022 (2023)
A Canetta, et al. Nano Letters 24, 6513-6520 (2024)
A Castellano, et al. Physical Review Materials 8, 084411 (2024)
D Ourdani, et al. Physical Review B 110, 014427 (2024)

A frozen-phonon approach to electron-phonon coupling in large supercells and heterostructures

Oliver Dicks, QMUL [contributed]

Electron-phonon coupling (EPC) governs a wide range of material properties, yet its calculation from first principles remains computationally prohibitive for the large and complex systems of greatest practical interest, including interfaces, heterostructures, and compounds with many atoms per unit cell.

We present an efficient method for estimating EPC from density functional theory calculations of frozen phonons, extracting coupling strengths from the perturbation of electronic bands near the Fermi energy in large supercells (https://github.com/od-qmul/lambda_calc_pub). We validate the approach against full Eliashberg calculations across a range of materials including hydrides, demonstrating good quantitative agreement. We further apply the method to interfacial systems such as MgO/TiO, where conventional approaches are intractable, demonstrating substrate enhancement of electron-phonon coupling modes.

Extending the accessible system size to ~1,000 atoms make realistic modelling of complex interfaces and heterostructures feasible for the first time within a DFT framework, opening new avenues for high-throughput screening of materials where electron-phonon interactions are central.

O. A. Dicks, K. Foyevtsova, I. Elfimov, R. P. Prasankumar, and G. Sawatzky, Phys. Rev. B 110, 184517 (2024)

Thermoelectric Transport Properties of Topological Surface States in Bi2Se3

Miguel Luque-Canete, King's College London [contributed]

Bi2Te3 and its alloys with Bi2Se3 and Sb2Te3 are the best performing thermoelectric materials near room temperature [1]. They are also topological insulators, exhibiting topological surface states (TSSs) with promising applications where understanding their electronic transport properties is essential [2].

At room temperature, electron-phonon interactions could significantly impact electronic and thermoelectric transport of TSSs, yet the dominant mechanisms of electron-phonon scattering remain unclear [3]. In this work, we develop and validate a framework to compute the phonon-limited transport properties of the TSSs in Bi2Se3 using the Boltzmann transport equation in the relaxation time approximation. We include scattering with acoustic and non-polar optical phonons via deformation potential coupling. Acoustic phonons are obtained from the anisotropic elastic continuum equations and non-polar optical phonons from an extended slab model [4]. We also introduce an anisotropic dielectric continuum model to account for long-wavelength optical phonon scattering. All physical parameters entering the framework are obtained from ab-initio calculations.

Applying the framework to the TSSs in Bi2Se3, we quantify scattering rates arising from distinct phonon modes and evaluate their contributions to the temperature-dependent transport properties.

Session 4: Excitons & photovoltaics

Phonon-Assisted Excited-State Dynamics in Semiconductors

Sivan Refaely-Abramson, Weizmann Institute of Science [invited]

Excited-state processes are essential for emerging applications in materials, from energy conversion to quantum information science. The associated generation and relaxation mechanisms are often coupled to quantum selection rules, stemming from the underlying material structure. In this talk, I will discuss the relation between excited-state evolution and structural design in low-dimensional semiconductors. I will present our band structure theoretical and computational approaches to calculate phonon-assisted exciton interaction dynamics as a function of the underlying structure and discuss the importance of many-body effects in the excited state relaxation and dephasing mechanisms. I will further discuss our ab initio – based data-driven approaches to explore excited-state relaxation upon phonon scattering, offering new design principles to achieve light-induced quantum coherence in semiconducting materials.

Intra- and interlayer excitons in a low-dimensional metal-halide perovskite

Linn Leppert, University of Birmingham [invited]

Excitons, neutral quasiparticles formed by electron-hole pairs, play a key role in the optoelectronic properties of semiconductors. Understanding their formation, transport, and dissociation is essential for interpreting experiments, predicting material behavior, and designing new materials for targeted applications. Low-dimensional halide perovskite semiconductors provide a versatile platform for studying excitons due to their structural tunability and ease of fabrication. Quasi-two-dimensional (2D) halide perovskites, consisting of metal-halide octahedral layers separated by organic spacers, are particularly promising. Their unique structure, which disrupts octahedral connectivity in one direction, results in anisotropic charge-carrier masses and dielectric screening, promoting the formation of strongly bound excitons.

First-principles calculations of excitonic properties in these materials have been limited by the large unit-cell sizes of most experimentally synthesized quasi-2D perovskites. However, recent advances in hardware and many-body perturbation theory methods, such as the GW and Bethe-Salpeter Equation approaches, now enable detailed insights into these systems. In this presentation, I will showcase how these calculations provide a microscopic understanding of the experimentally observed polarization dependence of intra- and interlayer excitons. Our results demonstrate that the fine structure of excitons in these materials is governed by crystal symmetry, the two-layer unit cell, and octahedral distortions, which can strongly enhance interlayer optical activity through mixing with intralayer excitonic states.

Anisotropic Optoelectronic Properties of a Newly Synthesised Quaternary Chalcohalide $CuSn_2SI_3$ from First Principles

Debalina Banerjee, Oxford University [contributed]

We present a first-principles investigation of the optoelectronic properties of the recently synthesised three-dimensional quaternary chalcohalide CuSn2SI3 [1], consisting of alternating layers of connected Cu-I and Sn-S-I polyhedra.

Density functional theory (DFT) calculations reveal a semiconductor with a direct band gap of approximately 1 eV. The electronic bands are dispersive along reciprocal space directions consistent with carrier transport along the Cu-I and Sn-S-I planes in real space but flat away from these planes for both the valence and conduction bands. This anisotropic band structure leads to direction-dependent effective masses. G0W0 calculations starting from PBE yield a quasiparticle band gap of 1.34 eV, while PBE0 and HSE calculations yield band gaps of 1.8 and 2.4 eV, respectively. For reference, experimental optical absorption spectra, reported in [1], exhibit an onset at 2.1 eV. Optical absorption spectra computed using the G0W0+BSE framework exhibit an absorption onset at approximately 1.45 eV, above the quasiparticle band gap, and reproduce the experimental absorption lineshape. We find weak optical transitions about 100 meV below the quasiparticle band gap, while the calculated optical spectrum does not exhibit excitonic resonances. Finally, we explore compositional trends across isostructural chalcohalides.

We acknowledge funding from the EPSRC, and computational resources from TACC (Frontera) and CINECA (Leonardo) with access via the Frontera Pathways and Euro-HPC programs respectively.

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Dielectric-dependent hybrid functional from meta-GGA

Stefan Riemelmoser, École Polytechnique Fédérale de Lausanne [contributed]

Semi local density functionals such as PBE typically underestimate experimental band gaps by 50%. Hybrid functionals address this "band gap problem" by admixing a fraction of Fock exchange to semi-local exchange. The optimal mixing parameter depends on the specific material and can be identified as the inverse dielectric constant [1].

Recently, we have shown that dielectric constants obtained using the r^{2}SCAN meta-GGA functional [2] are significantly more accurate than dielectric constants obtained using PBE [3]. Furthermore, a dielectric-dependent hybrid functional based on r^{2}SCAN can outperform the standard PBE-based hybrid in terms of band gaps [3]. Here, we showcase how the approximation for the DFT base functional relates to generalized Kohn-Sham and GW theories.

Furthermore, we will present recent applications to challenging materials, including narrow-gap semiconductors and strongly correlated transition metal oxides.

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Session 5: Photovoltaics & perovskites

Factors controlling charge pair generation in molecular semiconductors for photovoltaics

Jenny Nelson, Imperial College London [invited], Lucy Hart, Daniel Medranda, Linnea Lindh, Jolanda Muller, Hanbo Yang, Vanness Lai, Fabian Paehler, Mohammed Azzouzi, Flurin Eisner

The remarkable recent advances in photovoltaic energy conversion efficiency in molecular materials have resulted largely from the use of fused ring molecular acceptors that form strongly coupled domains in the solid state. These materials appear able to support efficient photocurrent generation with relatively small energetic offset between the ionization potential of donor and acceptor components, and the best performing molecular materials may even support charge pair generation in single material domains. In this work we investigate the behaviour of these materials by combining experimental measurements of charge generation in single-component and heterojunction devices with a computational model of the generation and evolution of delocalised excited states in such systems. We consider the influence of factors such as the nature of the charge separating heterojunction, molecular packing, energy and charge transport, electron-phonon coupling and loss pathways. We explore the impact of molecular parameters and find that low exciton reorganization energy and high and isotropic electronic coupling are important for efficient photogeneration. The same framework can be applied to polymer materials and tethered donor-acceptor structures. Finally, we will address the limits to energy conversion efficiency in such systems.

Molecular Engineering of Photogenerated Charge Transfer and Transport in Layered Hybrid Organic–Inorganic Perovskites

Kevin Sivula, École Polytechnique Fédérale de Lausanne [invited]

Layered hybrid organic–inorganic perovskites (LHOIPs) have emerged as a compelling platform for next-generation photovoltaic and optoelectronic devices, offering solution processability, structural tunability, and enhanced environmental stability relative to their three-dimensional counterparts. However, the quantum and dielectric confinement imposed by the organic spacer layers typically localizes photogenerated charge carriers within the inorganic slabs, limiting free carrier generation and out-of-plane transport.

A powerful strategy to address these limitations is the rational design of the organic spacer cation itself. Our group has shown that incorporating π-conjugated, electron-accepting naphthalene diimide (NDI)-based divalent or monovalent cations into the layered perovskite structure can create type-II nanoheterojunctions in which photogenerated electrons are transferred from the inorganic layer to the organic spacer on a picosecond timescale, as revealed by ultrafast transient absorption and fluorescence upconversion spectroscopy. This spatial separation of charges extends free carrier lifetimes and improves electron transport perpendicular to the layers, with out-of-plane electron mobilities reaching up to 0.1 $cm^2 V^{-1} s^{-1}$ as measured by space-charge-limited current methods.

Further tuning the light absorption and charge transport in these LHOIPs via molecular engineering presents significant challenges: the strong π–π interactions of bulky conjugated cations impede layered phase formation, and crystallinity is typically poor. Our group has developed strategies to overcome this, including optimization of alkyl linker chain length, solvent engineering, and a secondary spacer-assisted approach in which a small monovalent cation (e.g. phenylethylammonium) promotes nucleation of the NDI-based phase in the precursor solution, dramatically enhancing crystallinity and charge transport without forming a competing perovskite phase.

We further demonstrate that this design framework extends beyond lead-based systems to lead-free tin perovskites, and that tuning the organic dipole moment independently of interlayer spacing provides a route to systematically reduce exciton binding energies. Together, these results establish clear structure–function relationships linking molecular design, nanoscale heterojunction architecture, and photogenerated charge carrier dynamics in layered perovskites.

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Optoelectronic Properties of Organochalcogenide-Halide Perovskites from First-Principles

Austyn Masuno, University of Oxford [contributed]

Organochalcogenide-halide perovskites (RCh)PbX2 (RCh = NH3+(CH2)2S−, NH3+(CH2)2Se−; X = Cl−, Br−) have been recently synthesized and exhibit promising optoelectronic properties, making them attractive candidates for solar cell absorbers.1,2 In these new materials, the A-site cation and one of the X-site anions is replaced with a zwitterionic molecule, cysteamine or selenocysteamine, further expanding the optoelectronic landscape through the introduction of a chalcogenide into the perovskite framework.1,2 This new class of perovskites show enhanced structural stability to high temperature and pressure, while largely preserving many of the desirable optoelectronic properties and milder fabrication techniques of traditional halide perovskites.3

Following recent reports on the structural and electronic properties of these materials,1–3 we present a comprehensive GW+BSE first-principles study to investigate the excited-state properties of the (RCh)PbX2 perovskites. We report on quasiparticle band gaps, effective masses, optical absorption spectra, and exciton binding energies. We find exciton binding energies that are generally smaller than the lead-halide perovskite counterparts. This highlights these materials as promising candidates for efficient solar cell absorbers. Paired with experimental results, we see good agreement in the line shape of the optical absorption spectra, while not yet accounting for the compositional disorder. This study provides critical insight into the optoelectronic properties of this new family of materials, which will guide future efforts to improve their performance for solar cell applications.

Computational resources that have contributed to the research results reported here have been provided by the EuroHPC supercomputer LEONARDO, hosted by CINECA (Italy) and the LEONARDO consortium and the Texas Advanced Computing Center (TACC) at The University of Texas at Austin.

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Towards an understanding of triplet and charge formation in Y6 and YSe

Isabel Creed, Imperial College London [contributed]

The development of non-fullerene acceptors (NFAs) is an important step in the improved performance of organic photovoltaic devices (OPVs). One NFA of particular interest due to its unique photophysics is Y6. Y6 is reported to be able to generate free charges; a property often only observed at heterojunctions in OPVs. Additionally, it is of interest as a sensitiser molecule in Y6: Rubrene up conversion devices. These devices have an unusually high efficiency which Izawa and Hiramoto proposed was due to a new mechanism of up-conversion and are of interest as they are a way of improving OPV performance beyond the single-bandgap detailed-balance limit.

In our work, we examine the non-adiabatic dynamics of Y6 and YSe dimers based on an experimentally determined crystal structure of Y6, as the minimum model of the molecular crystals. We use an effective model Hamiltonian and Hierarchical Equations of Motion (HEOM) to examine the dynamics for times ranging from femto-nanosecond. We find that these Y6 and YSe dimers can rapidly form intermolecular charge transfer states on O(10fs), something we also see from other methods of examining the non-adiabatic dynamics. By contrast, the triplet states within the dimers only form on the O(1ns). We find that triplet state formation is facilitated through enhanced intersystem of the CT-FE states due to the change in symmetry of these states. By contrast, the FE-FE intersystem crossings matrix elements are extremely small as they are mainly transitions which are forbidden by El Sayed's rule.

Session 6: Organic materials

Charge Transport Physics of High Mobility Organic Semiconductors

Henning Sirringhaus, Cavendish Laboratory, University of Cambridge [invited]

Over recent years there has been tremendous progress in developing low-temperature, solution-processible organic semiconductors that provide high charge carrier mobilities for both n-type and p-type device operation, good operational stability and other functionalities such as efficient electroluminescene, sensing or memory functions for a variety of applications.

We are interested in understanding the spin and charge transport physics of these materials and the relationship between molecular structure, microstructure and spin and charge diffusion. In some state-of-the-art organic semiconductors structural disorder effects can be reduced to a level where it is becoming possible to study the more intrinsic limitations of charge transport in these materials and observe transport regimes that have hitherto not been accessible.

In this talk I will give an overview over the physics of molecular and polymer semiconductors and discuss their relevance for applications in large-area electronics.

From Light Absorption to Charge Separation: Exciton Delocalization and Coupled Electron-Nuclear Dynamics in Molecular Aggregates

Samuele Giannini, University of Pisa, Italy [invited]

Light absorption, charge separation, and electronic transport are vital for optimizing optoelectronic devices and designing new materials, yet a fundamental understanding remains challenging because these processes span multiple time, length, and morphological scales. Quantum phenomena, arising

from coupled electronic and nuclear degrees of freedom interactions (vibronic interactions), govern both the optical response [1,2] and electronic transport in supramolecular aggregates and organic semiconductors [3,4].

I will show how first-principles-based Hamiltonians, parametrized for realistic material morphologies and incorporating localized and charge transfer states, can explain aggregation-induced changes in steady-state optical spectra of non-fullerene acceptor molecules (NFAs) used in high-efficiency organic photovoltaics [1,2] and supramolecular aggregates for photocatalysis [5]. By coupling these Hamiltonians with both full quantum dynamics and mixed quantum–classical dynamics, we characterize the nature and evolution of electronic excitations across a broad range of timescales. Ultrafast dynamics in dense vibronic manifolds are resolved using efficient ML-MCTDH wavepacket propagation [5], while a new surface-hopping approach in the excitonic-state basis enables the determination of excited state dynamics and charge separation processes at longer times [4,6].

Our results clarify the role of exciton delocalization and coherence as well as electron-vibrational interactions in guiding the efficiency of important electronic processes such as charge separation in molecular aggregates [5,6] and provide structure–property relationships that inform the design of more efficient optoelectronic devices.

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Modelling the impact of molecular properties on charge generation in organic semiconductors

Lucy Hart, Imperial College London [contributed]

Through a remarkable series of advances in material design, the efficiency of organic solar cells has risen from 1% to over 20% within two decades, surpassing most predictions. Key to reaching this milestone has been the development of nonfullerence acceptors (NFAs) which, when paired with suitable polymer donors, yield high internal quantum efficiencies (IQEs) despite having a significantly smaller driving force for exciton splitting than is present in typical polymer: fullerene systems. There is some evidence that the best performing NFAs can generate charge separated states within single material domains, and it has been suggested that this process is what underlies their ability to efficiently generate charge pairs across a heterojunction. In this work, we address this question using an experimentally validated computational model of charge pair generation in molecular crystals. Our model can account for the significant effects of excitonic and electronic delocalisation on both excited state lifetimes and on charge and energy transfer rates. Using this model, we track the time evolution of excited states in single-component systems and demonstrate how both intramolecular parameters, such as reorganisation energy, and intermolecular parameters, such as electronic coupling, influence the yield of charge separated states. By analysing our results within a thermodynamic framework, we can identify the main loss pathways and thus identify the states which limit the overall yield of free charges. Additionally, we investigate how the same set of parameters affect charge generation efficiency in heterojunctions. Our results indicate that, although there is a correlation between the ease of charge generation in single-component and heterojunction systems, it is unlikely that charge pairs generated in the acceptor domains contribute significantly to the photocurrent in a heterojunction architecture.

A Radical Approach to Machine Learning and Electronic Structure Theory

Tim Hele, University College London [contributed]

Recent years have seen an explosion of interest in organic radicals due to their high efficiency in organic light-emitting diodes (OLEDs) and for use in qubits. However, modelling their electronic structure is challenging due to the large size of the molecules, their multireference electronic structure, and the spin contamination problem which can arise from multiple unpaired electrons in the excited states.

In this presentation I will present ExROPPP, which we believe is the fastest known method for radical excited state computation, has accuracy comparable to high-level multiconfigurational calculations, and in spin-pure [1]. In addition, alternacy or pseudoparity rules for ground-state closed shell radicals had been derived in the 1950s by Pariser, Parr and Pople but there was no extension to radicals due to the algebraic complexity. In deriving ExROPPP we (Green and Hele) also derived alternacy or pseudoparity rules for the excited states of hydrocarbons radicals, showing their excited states also have 'plus' and 'minus' forms [1].

I will then show what we believe is the first example of machine learning directly from the excited states of radicals where we extend ExROPPP to molecules also containing nitrogen and chlorine by learning the optimal parameters from experimental absorption data and molecular structures [2]. These breakthroughs pave the way for the high throughput discovery of the next generation of radical-based optoelectronics.

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Day 3 - 3 June 2026

Session 7: Thermoelectric materials & electron-phonon interactions

Optimizing Thermoelectric Materials: Balancing Performance, Cost, and Sustainability

Maria Ibanez, Institute of Science and Technology, Austria [invited]

Advancing thermoelectric technology requires more than chasing ever higher zT values; it demands a rethink of how we design, synthesize, and manufacture materials. Colloidal chemistry and extrusion-based 3D printing offer a powerful combination: the former enables precise control over material composition and microstructure through solution-based routes, while the latter provides a flexible platform for shaping materials into device-ready architectures with minimal waste and energy input. Together, they open a new space for engineering thermoelectric materials that are not only high-performing but also scalable and sustainable. In this talk, I will discuss how interfacial chemistry, ink formulation, and porous microstructures can be harnessed to create functional materials with excellent charge and phonon transport, challenging the assumption that high performance requires high density or high-temperature processing. This approach can be broadly applicable, and I will highlight how it can be adapted beyond traditional systems to inspire new strategies for thermoelectric integration and fabrication.

Electronic transport calculations in the search for high power factor thermoelectric materials

Neophytos Neophytou, University of Warwick [invited]

Advances in materials synthesis and chemistry have enables the realization of numerous novel materials and their alloys, many of them with complex electronic structures and transport features. Here I present an efficient fully ab initio computational method that we have developed, in order to calculate electronic and thermoelectric properties of such materials. The method is formulated in the Boltzmann Transport code Electra, which is publicly available. Using this, I will present studies of transport in complex materials such as half- and full-Heuslers, and Mg3Sb2, and metallic materials, and their alloys, all of which are prominent thermoelectric materials. I discuss optimization directions for their thermoelectric power factor by identifying favourable electronic structure features. Scalability and accuracy further allows the extraction of test sets that serve machine learning purposes, and in this context, I will present the development of effective descriptors that allow fast scan of a large number of materials and their alloys for electronic conductivity and power factor.

Minimizing the Lorenz number via Energy-Selective Transport

Illia Serhiienko, TU Wien [contributed]

In metallic thermoelectrics, the figure of merit reduces to zT≈S^2/L in the electron-dominated regime. While thermoelectric optimization still relies primarily on enhancing the Seebeck coefficient S, the Lorenz number L becomes the second key parameter controlling performance. Yet comparatively little attention has been paid to strategies for suppressing L below its Sommerfeld value. Within the

Boltzmann transport, L can be expressed in terms of the variance of carrier energies relative to the chemical potential, $L \sim \mathrm{Var}(E - \mu)$, implying that narrowing the energy distribution of conducting carriers provides a direct route to lowering L.

Here, we develop a general framework for energy-selective transport in metals and show how strongly energy-dependent scattering can be used to control the Lorenz number. Building on recent observations of enhanced thermopower in Ni3Ge [1] and Ni3In [2], we identify a common principle: interband scattering with strong energy dependence creates an effective transport window, leading to enhanced carrier asymmetry and an increased Seebeck coefficient. This behaviour is promoted by flat-band features in the electronic structure, which strongly modify the scattering phase space near the Fermi level. We further extend this concept to systems hosting two flat bands separated by an energy scale W.

We show that such a configuration can generate a boxcar-like transport distribution function, selectively suppressing carrier contributions outside a narrow energy window. This reduces Var(E - μ) and thus suppresses the Lorenz number significantly below its Sommerfeld value without strongly compromising the electrical conductivity. These results establish energy-selective transport engineering as a general strategy for approaching the ideal transport distribution in metallic thermoelectrics.

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Coupled electron-phonon hydrodynamics and Viscous Thermoelectric Equations

Bogdan Rajkov, University of Cambridge [contributed]

Non-diffusive, fluid-like transport of charge and heat has been observed in several materials, raising the question of whether they can emerge simultaneously and how they are related to electron-phonon bifluids.

Here we introduce a first-principles theory and computational framework to quantitatively describe these phenomena from atomistic to continuum scales in complex device geometries. Starting from the microscopic coupled electron-phonon Boltzmann transport equation, we formalize the emergence of composite “relaxon” electron-phonon excitations, show that they determine the viscosity tensors of the two fluids, and quantify the impact of electron-phonon drag on thermoelectric transport coefficients. We then demonstrate that the coupled Boltzmann equation can be coarse-grained into a set of mesoscopic Viscous Thermoelectric Equations, formally unifying Gurzhi’s hydrodynamic equation for electrons [Sov. Phys. Usp., 1968] and the recently developed Viscous Heat Equations for phonons [PRX 10, 011019, 2020], while extending them to cover the intermediate regime of mixed electron and phonon fluids. We leverage this framework to elucidate how electron and phonon fluids can coexist or mix, rationalizing pioneering experiments on electron-phonon drag in graphite, and predicting smoking-gun signatures of non-diffusive behaviour such as non-harmonic temperature and electric potential fields, and compressible thermoelectric backflow.

Path integral polarons for real semiconductors

Jarvist Frost, Imperial College London [contributed]

Most technically relevant behaviours of semiconductors for energy materials are emergent phenomena. Rather than being direct quantum observables, they arise due to the competition between different, similar strength, processes, and are transient and finite-temperature. This poses a considerable challenge for materials modelling

A particular recent focus of ours has been the charge-carrier mobility in polar semiconductors. The charge-carrier polarises the lattice, and the back-reaction attempts to localise the charge carrier. Truly this is a finite-temperature quantum field-theory problem (as phonons can be created and destroyed). Most modelling is limited to semi-classical rate theory-based models (such as Marcus theory; Boltzmann transport equation).

Our computational tool of choice is the Feynman path integral variational approximation. Once the model Hamiltonian parameters are set by electronic structure calculations on the material of interest, we use this finite-temperature quantum-field-theory theory to make direct quantitative predictions of finite temperature charge-carrier response in both inorganic and organic semiconductors.

We extended the Feynman variational method for the solid-state Froehlich Hamiltonian to multiple phonon modes and multiple quasiparticles in the variational solution and developed the numerics to predict finite-temperature frequency-dependent observables (particularly optical absorption and polaron mobility), of more complicated multi-phonon branched semiconductors as are often proposed as future inorganic photovoltaic materials [PRB 107 115203].

We developed a Feynman variational method for the Holstein Hamiltonian, allowing us to use the same machinery to simulate 'small' polarons in organic materials [arXiv: 2207.06846]. Finally, I will describe how this picture of the Feynman dynamic polaron localisation can be used to correct quantum scattering form-factors that otherwise rely on (incorrectly) fully delocalised Bloch waves [unpublished].

[PRB 107 115203] https://doi.org/10.1103/PhysRevB.107.115203 [arXiv: 2207.06846] https://arxiv.org/abs/2207.06846

Session 8: Nanoplasmonics

Visualizing and Designing Energy Flow in Nanomaterials

Emiliano Cortés, Ludwig Maximilian University of Munich [invited]

Understanding and controlling the generation, transport, and storage of energy at the nanoscale is key to developing sustainable energy technologies. Our work brings together rational materials design with state-of-the-art imaging and spectroscopic tools to probe and direct energy flow in a broad range of functional nanomaterials [1-10].

In the first part of the talk, I will discuss our strategies for designing plasmonic, photonic, and photocatalytic materials capable of capturing light and converting it efficiently into chemical energy. By synthesizing precisely tailored nanostructures, we investigate the fundamental processes that govern solar-driven hydrogen production and carbon dioxide reduction, with the goal of defining design rules for scalable energy conversion systems.

In the second part, I will present new imaging and characterization approaches that make it possible to monitor charge and energy dynamics in real time with nanometre-scale resolution. These methods are not limited to light-harvesting materials, but also apply to light-emitting, catalytic, battery, and two-dimensional systems, offering powerful opportunities for imaging-guided optimization of material performance.

By connecting structure, dynamics, and reactivity across different classes of materials, this talk will outline a unified framework for the design of efficient and sustainable systems for energy harvesting, conversion, and storage. More broadly, this integrated perspective strengthens our ability to visualize, control, and optimize energy flow from the atomic scale to practical applications.

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Modelling of hot electron dynamics in plasmonic nanoparticles for photocatalysis

Leonardo Biancorosso, University of Trieste [contributed]

In recent years, plasmonic materials have attracted growing interest across a wide range of technological applications, from photocatalysis to sensing. As their use continues to expand, a thorough understanding of the underlying physical and chemical processes becomes essential to effectively model and engineer these materials for enhanced performance. A key mechanism in this context is hot carrier generation [1]: upon illumination, plasmon modes excited on the nanoparticle surface decay through Landau damping, producing energetic electrons and holes that can drive chemical reactions under milder conditions than in traditional thermal catalysis [2,3]. In this framework, properly capturing the coupling between plasmonic materials and molecular systems or other interfaces becomes critical, as these interactions span multiple length and time scales. Addressing this complexity requires a multiscale modelling approach capable of treating the different degrees of freedom of the system within a unified framework [4].

In this work, we present an effective methodology to study the electronic response of molecular systems by performing electronic dynamics simulations in the presence of plasmonic metal nanoparticles to elucidate how the local plasmonic environment influences the behaviour of adsorbed molecular systems in relevant photocatalytic processes [5]. We further advance the understanding of these phenomena by systematically investigating how the size and geometrical configuration of the nanoparticles affect hot-carrier generation and discuss the implications for the rational design of plasmon-assisted photocatalytic systems [6].

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Modelling plasmon-induced vibrational dynamics of adsorbates on metal nanoparticles

Chengcheng Xiao, Imperial College London [contributed]

Plasmonic nanoparticles are typically noble metal nanoparticles (NPs) that exhibit a unique optical phenomenon known as localised surface plasmon resonance. These surface plasmons can be utilised to drive surface chemical reactions, leading to a new paradigm of light-driven catalysis that is more energy efficient and environmentally friendly than traditional thermal-driven chemical reactions. One of the key components in studying light-driven catalysis using plasmonic NPs is the process of energy transfer from the plasmonic NPs to adsorbed molecules.
Understanding this process can help design more efficient catalytic reactions. A model reaction for this process is the nitro-reduction of 4-nitrobenzenethiolate (4NTP) to 4,4-dimercaptoazobenzene (DMAB) on silver NPs under illumination.

In this talk, we discuss how plasmon-generated hot carriers induce vibrational dynamics in the 4NTP molecule. Specifically, we model hot-carrier injection into the molecules and how this affects the vibrational properties of the molecules, which can be measured using surface-enhanced Raman spectroscopy. We find that hot-electron injection can explain the observed intensity enhancement of the N=O symmetrical stretching mode, which plays an important role in the nitro-reduction reaction. Next, we study the transfer of energy from this mode into the N=O scissoring mode through a three-phonon process and compare this process in 4-NPT and the fluorinated 4NPT molecules, finding good agreement with experimental measurements.

Our results shed light on how surface plasmon-induced hot electrons affect the vibrational properties of adsorbed molecules and how altering certain molecular traits can give rise to large changes in the vibrational interactions, which helps the design efforts of novel light-driven reduction reactions.

High-throughput first-principles screening of surface work functions for water splitting applications

Francesca Martini, University of Trento [contributed]

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, 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 semi local 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 work function 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.

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

Session 9: Machine learning for energy

Data Generation, Heuristics, and Machine Learning for Materials Discovery and Simulation

Janine George, University of Jena [invited]

Machine learning (ML) offers powerful new strategies for accelerating the discovery and design of functional materials. In our work, we develop ML models and software frameworks for large-scale screening and advanced materials simulations, starting from robust high-throughput quantum-chemical workflows, such as those implemented in atomate2.[1,2] These automated workflows enable the creation of large, high-quality materials databases that form the foundation for data science and machine learning. In addition to experimentally known crystal structures, increasingly generative models are used to extend materials databases, which also need to be evaluated.[3]

To build predictive, scientifically grounded ML models, we use chemical bonding concepts, incorporating quantum-chemical bonding strengths and related descriptors as physically meaningful features to predict vibrational properties and heat transport.[4,5] Beyond property prediction, we address the challenge of determining which hypothetical materials are synthesizable. To this end, we introduced co-training into a positive–unlabelled (PU) learning framework, enabling ML-based classification even in the absence of true negative data—an essential step for screening synthesizable compounds.[6,7]

To advance atomistic simulations of complex materials, we further developed automated training pipelines for ML interatomic potentials that support both general-purpose and system-specific potential development, as implemented in our software autoplex.[8] This automated approach has already facilitated detailed investigations of challenging systems, including the computational exploration of amorphous arsenic.[9]

Together, these developments provide a toolbox spanning workflow automation, automated ML potential training, and ML models for materials properties and synthesis, enabling scalable, data-driven discovery and understanding of advanced materials.

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Machine learning for materials science; a bittersweet lesson

Keith Butler, University College London [invited]

According to Rich Sutton in his influential essay *The Bitter Lesson*, "researchers seek to leverage their human knowledge of the domain, but the only thing that matters in the long run is the leveraging of computation." This stark claim runs counter to the instincts of most practicing scientists, for whom domain knowledge and inductive biases have a privileged status. In this talk I will explore how applicable Sutton's Bitter Lesson is to research in computational materials science, drawing on some recent research from our group. I will show how, in certain situations where data is plentiful and covers the domain of application, large models, with loose inductive biases prove (surprisingly) successful. On the other hand, I show how using physics in the process of model design allows us to capture responses of the system that were never exposed during training, hopefully demonstrating that there is still a place for human intelligence in materials modelling, and providing a sweet aftertaste to the bitter lesson.

Simulating electrochemical interface under explicit bias: ab initio and machine learning

Jing Yang, Imperial College London [contributed]

Ab initio molecular dynamics (AIMD) serves as powerful method for studying the electrochemical processes at solid/liquid interfaces. To drive these surface reactions, a macroscopic electric field needs to be applied to the system, which is a major source of computational complexity. For these calculations, there exists multiple methods with different treatments of the counter charges and the boundary conditions, some of which are not necessarily included in standard DFT codes. In addition, the AIMD calculations are often prohibitively expensive for observing the reaction process in real time. Machine learning interatomic potentials (MLIPs) offer the promise of a much cheaper alternative, but the accuracy of such potentials for describing long-range electrostatic interaction is still questionable. In this talk, we first discuss the implementation for calculating electrified surface under arbitrary field by utilizing the newly released VASP-python interface. This development allows one to perform AIMD with applied electric field using the standard VASP code with great control and flexibility. Next, we discuss some of the recent developments of machine learning potentials with long-range electrostatic interaction. We show that ML models that are trained on local charge distributions, such as Hirshfeld charge or Wannier centers, do not necessarily reproduce the macroscopic electrostatics. We propose a model which is instead trained on the macro dipole moment and show that such a model can predict the macroscopic electric field for realistic electrochemical systems.

Data-Driven Design of Photovoltaics, Thermoelectrics and Transparent Conductors

Ruiqi Wu, Imperial College London [contributed]

The discovery of new materials has driven advances in energy conversion and storage, including batteries, photovoltaics, thermoelectrics and transparent conductors. Recently, Google released the GNome dataset of hypothetical compounds, built on an unbiased screening of chemical space, which identified thousands of novel, potentially stable inorganic materials. However, the true stability of these compounds remains unclear, and their functional properties have yet to be evaluated for energy applications. In this work, we carry out a large-scale high-throughput screening of the GNome dataset. We employ hybrid density functional theory to robustly evaluate the optoelectronic properties of over 600 compounds, selected according to their earth-abundant and non-toxic compositions and predicted bandgaps. Based on this, we ranked the compounds based on their suitability for photovoltaics, thermoelectrics and transparent conductor applications. To provide reliable predictions of materials stability, we comprehensively ensure the predicted materials are the true thermodynamic ground state through ab initio random structure searching, while dynamical stability is assessed through vibrational properties. For the most promising candidates, we obtain the intrinsic defects and electronic transport properties to guide experimental device design. Our work identifies several novel earth-abundant candidates with state-of-the-art performance in energy applications.

Data Driven Screening of Dopants for Functional Materials

Ahmed Ismail, University College London [contributed]

Currently the vast majority of materials design and generative models focus of proposing perfect crystals as candidates for specific applications; this paradigm neglects the critical role of dopants for real-world materials' functionality. Dopant engineering plays a central role in tailoring the electronic, optical, and functional properties of inorganic materials used in applications such as ferroelectrics, catalysis, transparent conducting oxides, and energy technologies. However, identifying suitable dopants remains a challenging problem because the number of possible host–dopant combinations grows rapidly with chemical complexity. Systematically evaluating these possibilities using first-principles calculations, such as density functional theory (DFT), is computationally demanding and often impractical for large chemical spaces. The problem gets exponentially worse when common strategies such as co-doping are considered. As a result, efficient strategies are required to reduce the search space while maintaining reliable predictions of material stability and functionality.

In this work, a data-driven workflow is developed to accelerate dopant discovery by combining rule-based chemical screening with data-driven atomistic modelling. Candidate dopants are initially screened using the SMACT [1] framework, which evaluates chemical feasibility based on oxidation states, charge neutrality, ionic size compatibility, and chemical similarity metrics. The resulting chemically plausible substitutions are then evaluated using machine-learned interatomic potentials, specifically the MACE model [2], enabling rapid estimation of energetic trends for doped structures at a fraction of the cost of conventional DFT calculations. Promising candidates are subsequently validated through DFT simulations to confirm energetic stability and structural relaxation. We perform a statistical analysis of the results from heuristic screening, data driven potentials and DFT calculations, demonstrating that there is a strong rank correlation between suggested candidates from each level of the screening process. This allows us to establish this workflow as a robust method for high-throughput design of doping strategies tailored to specific materials and represents an important step towards computational design of materials for real-world applications.

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