MM 31: Transport in Materials: Diffusion, Charge, or Heat Conduction II

Time: Thursday 10:15–13:00 Location: SCH/A216

MM 31.1 Thu 10:15 SCH/A216

Thermal Transport through Benzene-1,3,5-Trisamide Fibers — •Eberhard Lukas Flöter and Fabian Pauly — Universität Augsburg, Augsburg, Germany

Benzene-1,3,5-trisamides (BTAs) are a group of chiral and polar molecules which consist of a benzene ring, three amide groups and various side groups. Hydrogen bonding between the amide groups lets the BTAs assemble to columns. These columns pack into hexagonal structures, forming fibers. Since BTAs are chiral and polar, there are multiple configurations that these structures can take. We use nonequilibrium molecular dynamics (NEMD) methods and force fields to model thermal transport through BTA fibers in various configurations. In the presentation we discuss how thermal transport depends on side groups, molecular stacking and defects.

MM 31.2 Thu 10:30 SCH/A216

Phonon Interference in Single-Molecule Junctions — Sai C. Yelishala[1], Yunxuan Zhu[1], •Pablo M. Martinez[2,3], Hongxuan Chen[4], Mohammad Habibi[1], Giacomo Prampolini[5], Juan Carlos Cuevas[3,6], Wei Zhang[4], Guilherme Vilhena[2], and Longji Cui[1,7] — [1]Paul M. Rady Department of Mechanical Engineering, University of Colorado Boulder, USA — [2]Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), Spain. — [3]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Spain. — [4]Department of Chemistry, University of Colorado Boulder, USA — [5]Istituto di Chimica dei Composti Organo Metallici (ICCOM-CNR), Italy. — [6]Condensed Matter Physics Center (IFIMAC), Spain — [7]Materials Science and Engineering Program and Center for Experiments on Quantum Materials, University of Colorado Boulder, USA.

Wave interference opens a new route to control transport properties and has been widely studied in electronic and photonic materials. However, interference of phonons, which govern thermal transport in insulators, has been poorly characterized due to experimental challenges. We report the observation of phonon interference at room temperature in molecular-scale junctions. This is enabled by custom-developed scanning thermal probes which can track heat flowing through a single molecular junction at a time. Using isomers of oligo(phenylene ethynylene)3 with either para- or meta-connected centre rings, we reveal a 40% reduction in thermal conductance for the latter. Quantum-mechanically accurate simulations show this difference arises from the destructive interference of phonons through the molecular backbone.

MM 31.3 Thu 10:45 SCH/A216

Phunky.jl - A Multithreaded Phonon Spectral Function Calculator In Julia — •William L. Wenig and Nakib H. Protik — Humboldt-Universität zu Berlin, Berlin, Germany

The ability to compute the phonon properties of materials is crucial for the understanding of physical phenomena such as transport and spectroscopy. At present, several code packages exist that allow ab initio access to phonon computations. These codes are mostly written in traditional languages such as Python, Fortran, or C++. In this talk we present Phunky.jl, a new tool for computing the harmonic and anharmonic phonon properties of materials. The tool is written in Julia, a language that has been designed specifically for scientific computation. It allows researchers to write software at a high level of abstraction, while generating code that runs at speeds faster or comparable to that of more traditional languages in this domain. Phunky.jl is written in an extensible manner so that one can easily expand and interface it with phonon transport solvers. We will highlight the capabilities of Phunky.jl by calculating the phonon spectral quantities for a selection of materials.

MM 31.4 Thu 11:00 SCH/A216

Understanding How Pressure Enhances Heat Transport in Organic Semiconductors — •Lukas Legenstein[1,2], Sandro Wieser[1,3], Michele Simoncelli[4], and Egbert Zojer[1] — [1]Graz University of Technology, Austria — [2]Montanuniversität Leoben, Austria — [3]TU Vienna, Austria — [4]Columbia University, USA

Understanding how lattice thermal conductivity changes under pressure is increasingly important in materials science, yet difficult to predict because materials exhibit a variety of behaviors, ranging from monotonic increases or decreases to anomalous trends. Molecular crystals, including organic semiconductors, stand out for exhibiting unusually large pressure-induced increases relative to their (ultra-)low thermal conductivities.

Our test system, naphthalene, crystallizes in a herringbone stack, a packing motif common in most π-conjugated organic semiconductors. Measurements up to 2 GPa from previous literature show an isotropic thermal conductivity that is up to four times higher than at ambient conditions. By combining highly accurate machine-learned potentials with the Wigner transport equation, we not only reproduce these findings but also elucidate how compression affects naphthalene's anisotropic thermal conductivity and how phonon tunneling becomes less relevant with increasing pressure. Finally, we trace the pressure-induced enhancement to frequency upshifts and the associated modifications in phonon scattering.

MM 31.5 Thu 11:15 SCH/A216

Building Trust in Ab Initio Machine-Learning Potentials for Extreme Materials – Applications to Strongly Anharmonic Ceramics and Thermal Insulators — •Shuo Zhao[1], Kisung Kang[1,2], and Matthias Scheffler[1] — [1]The NOMAD Laboratory at FHI, Max Planck Society — [2]School of Materials Science and Engineering, Chonnam National University

Thermal insulating ceramics and semiconductors often exhibit significant anharmonicity, particularly associated with rare events such as Frenkel defect creation and rattling phonon modes. These phenomena not only disrupt the phonon picture and the conventional perturbative methods for heat transport, but also pose challenges for the effective and trustful training of machine-learned interatomic potentials (MLIPs). Our contribution describes the implementation of a framework that combines the non-perturbative Green-Kubo formalism with a sequential, uncertainty guided active learning scheme using `AlmoMD`[1] with equivariant neural networks `NequIP`[2] and `So3krates`[3]. The approach is demonstrated by application to possibly ultra-low thermal conductivity materials[4]. Our results not only substantiate reliable predictions of thermal conductivity for strongly anharmonic systems but also pave the way for the accelerated exploration and design of novel thermal insulators.

[1] K. Kang, *et al.*, *Phys. Rev. Mater.* **9**, 063801 (2025). [2] S. Batzner, *et al.*, *Nat. Commun.* **13**, 2453 (2022). [3] J.T. Frank, *et al.*, *Nat. Commun.* **15**, 6539 (2024). [4] T.A.R. Purcell, *et al.*, *Npj Comput. Mater.* **9**, 112 (2023).

15 min. break

MM 31.6 Thu 11:45 SCH/A216

Probing Lattice Anharmonicity and Thermal Transport in Ultralow-κ Materials Using Machine Learning Interatomic Potentials — •Soham Mandal[1], Ashutosh Srivastava[2], Tanmoy Das[1], Abhishek Singh[2], and Prabal Maiti[1] — [1]Centre for Condensed Matter Theory, Department of Physics, Indian Institute of Science, Bangalore 560012, India — [2]Materials Research Centre, Indian Institute of Science, Bangalore 560012, India

Crystalline solids with ultralow lattice thermal conductivity (κ) are promising candidates for thermoelectric and thermal-barrier applications, yet understanding heat transport in such strongly anharmonic systems remains challenging. Perturbative frameworks such as the Boltzmann transport equation (BTE) are unreliable when anharmonicity is large and higher-order phonon scattering cannot feasibly be computed. Here, we develop machine-learning interatomic potentials (MLIPs) to study heat transport in TlAgSe and $Cs_2PbI_2Cl_2$ and compare three transport formalisms: Green-Kubo (GK), BTE, and the Wigner transport equation (WTE). BTE underestimates κ, while WTE improves agreement but slightly overpredicts due to neglected higher-order scattering. The non-perturbative GK framework captures full anharmonicity and closely matches the experimental κ value. Phonon scattering rates exceeding the Ioffe-Regel limit and the degree of anharmonicity $\sigma^A > 0.5$ confirm the strongly anharmonic nature of both materials. This MLIP-integrated framework advances predictive understanding of ultralow-κ heat transport and supports future materials design.

MM 31.7 Thu 12:00 SCH/A216

Current-voltage curves of transformer oils: Analytical and numerical results — •Markus Bier — Technische Hochschule Würzburg-Schweinfurt, Schweinfurt, Germany

High-voltage transformers contain oil, which should allow for convective heat transport while sustaining electrical insulation. These oils are complex fluids composed of various molecular and colloidal species which, over time, give rise to the formation of charged entities due to numerous, by now not entirely known and fully understood mechanisms. A widely used technique to diagnose transformer oils are current-voltage curves, which can exhibit remarkable and non-trivial transient features upon polarisation of a relaxed oil or repolarisation of an electrically stressed oil. Theoretical modelling provides a bottom-up approach to link current-voltage curves to the underlying charge transport processes. The present contribution reports on analytical and numerical results obtained within theoretical investigations of reaction-drift-diffusion models based on Poisson-Nernst-Planck (PNP) theory. After presenting an analytical solution of the PNP equations for a semi-infinite system in the non-equilibrium steady state as well as analytical cross-over boundaries between different repolarisation regimes, the main features of numerical transient current-voltage curves for polarisation and repolarisation are discussed.

Reference: M. Bier, "Non-equilibrium steady states of electrolyte interfaces", New J. Phys. 26, 013008 (2024).

MM 31.8 Thu 12:15 SCH/A216

Interband effects in the matrix Boltzmann transport equation — •Elena Trukhan and Nakib H. Protik — Department of Physics and CSMB, Humboldt University of Berlin

The current state-of-the-art ab initio method for computing electronic transport properties relies on the Boltzmann transport equation (BTE). However, the BTE fails to capture certain quantum effects, most notably interband coherence. To address this limitation for phonon transport, Simoncelli et al [1]. developed an approach based on the Wigner transport equation, which incorporates these effects by including the off-diagonal terms of the density matrix. This framework was later adapted to electrons by Cepellotti and Kozinsky [2]. Their method, however, involves several critical simplifications; for instance, it ignores kinetic corrections and treats the collision integral within a relaxation time approximation (RTA). Also, modern derivations rely on the assumption of a band-diagonal form of the interaction self-energies, which might not hold generally. In this work, we derive a more general electronic transport equation from a Green's function formalism. Using a modified Kadanoff-Baym Ansatz, we carefully track the terms that survive various standard approximations in the Dyson equations in the band representation, explicitly include electron-impurity and electron-phonon interactions, keeping self-energy in non-diagonal form and present a framework that captures interband coherence while moving beyond the RTA.

[1] M. Simoncelli, et al., Phys. Rev. X 12, 041011 (2022) [2] A. Cepellotti and B. Kozinsky, Mater. Today Phys. 19, 100412 (2021)

MM 31.9 Thu 12:30 SCH/A216

Coulomb and phonon scattering limited transport in doped systems — •Nakib H. Protik and Dwaipayan Paul — Humboldt-Universität zu Berlin, Berlin, Germany

In this talk we present an extension of the elphbolt [1] transport code package that includes the Coulomb interactions among the charge carriers. We perform ab initio calculations to study the effect of these interactions on the transport properties of doped systems over a range of temperatures. Specifically, we probe the charge carrier hydrodynamics in these systems and identify the relative roles of the Coulomb and phonon scattering in the realization these transport regimes. We provide a comparison with recent measurements and comment on the violation of the Wiedemann-Franz law.

[1] N. H. Protik, C. Li, M. Pruneda, D. Broido, and P. Ordejón, The elphbolt ab initio solver for the coupled electron-phonon Boltzmann transport equations, npj Computational Materials 8, 28 (2022).

MM 31.10 Thu 12:45 SCH/A216

Stoichiometric Locking in the High State of Charge in Solid Ion Conductors: A Kinetic Monte Carlo Study — •Roya Ebrahimi Viand, Chiara Panosetti, Christoph Scheurer, Karsten Reuter, and Sebastian Matera — Fritz-Haber-Institut der MPG, Berlin

The advancement of solid-state batteries critically relies on a deep understanding of ion transport in crystalline electrolytes and electrode active materials. We present a kinetic Monte Carlo (kMC) approach with fast update rules for transition propensities that enables efficient simulation of systems with long-range Coulomb interactions. Our study systematically probes the effects of state of charge (SOC), temperature, and applied external electric field on ionic mobility. We observe a pronounced mobility minimum near 100% SOC, where ions freeze in a low-energy Coulomb superlattice configuration that persists even under applied electric fields. Deviations from stoichiometry dramatically enhance transport by introducing defect pathways, with nearly symmetric behavior for ion and vacancy diffusion. By decomposing the state of charge into a reference and an excess carrier concentration (ΔSOC), we find that the intrinsic mobility per excess carrier remains approximately constant across different SOC values, revealing that transport is fundamentally mediated by the ΔSOC disrupting the reference structure. Analysis of effective activation energies across different SOC values reveals behavior consistent with percolation-controlled transport, where the availability of defect-mediated pathways strongly influences the energy landscape for ion diffusion.