MM 21: Transport in Materials: Diffusion, Conduction of Charge or Heat I

Time: Tuesday 10:15–11:30 Location: C 264

MM 21.1 Tue 10:15 C 264

Transport and diffusion in the two-dimensional Hubbard model — •Martin Ulaga[1], Jernej Mravlje[1,2], Peter Prelovšek[1], and Jure Kokalj[3,1] — [1]Insitute "Jožef Stefan", Ljubljana, Slovenija — [2]Faculty of mathematics of physics, University of Ljubljana, Ljubljana, Slovenija — [3]Faculty of civil and geotedic engineering, University of Ljubljana, Ljubljana, Slovenija

We study transport coefficients and diffusion constants in the square lattice Hubbard model by using the finite-temperature Lanczos method and Nernst-Einstein relations. Notably, we observe a strong, non-monotonic temperature dependence in heat conductivity that violates the Mott-Ioffe-Regel limit across a wide range of parameter space, mirroring the behavior of charge conductivity. These findings are particularly significant for experiments on cold-atomic gases, as well as on cuprates. We comment on the experimental implications of our results for thermal conductivity in the Mott-insulating regime and the Lorenz ratio in the doped Mott insulator.

MM 21.2 Tue 10:30 C 264

Transport mechanism in Lithium thiophosphate — •Davide Tisi, Lorenzo Gigli, Federico Grasselli, and Michele Ceriotti — Ecole Polytechnique Federale de Lausanne (EPFL)

Lithium ortho-thiophosphate (Li3PS4) are a promising candidate for solid-state-electrolyte batteries. The microscopic mechanisms of Li-ion transport in Li3PS4 are, still, far from being fully understood, and no computational work has tackled the thermal conductivity at DFT level.

In this talk, I will show how we build multi-level machine learning potentials targeting state-of-the-art DFT references (PBEsol, SCAN, and PBE0), to study the electrical and thermal conductivity of all the known phases of Li3PS4 (α, β and γ). I will discuss the physical origin of the superionic behaviour of Li3PS4: the activation of PS4 flipping drives a structural phase transition to a highly conductive phase, characterised by an enhancement of Li-site availability and by a drastic reduction in the activation energy of Li-ion diffusion. I will show the effects of the phase transition on both the electrical and thermal conductivity. We elucidate the role of inter-ionic dynamical correlations in charge transport, by highlighting the failure of the Nernst-Einstein approximation to estimate the electrical conductivity. Finally, we compare the thermal conductivity computed by the Green-Kubo theory with the results from the Boltzmann transport equation, to highlight the role of anharmonicity and quantum effects.

Our results show a dependence on the target DFT reference, with PBE0 yielding the best quantitative agreement with experiments.

MM 21.3 Tue 10:45 C 264

Phonon anharmonicity at lower mantle conditons: Consequences on the thermal conductivity of MgO — •Saadi Chabane, Paola Giura, Lorenzo Paulatto, and Daniele Antonangeli — Institut de minéralogie, de physique des matériaux et de cosmochimie, Sorbonne université, Paris, France

Understanding the properties of Magnesium oxide's (MgO) properties is essential for planetary sciences and technology, especially as a fundamental component in Earth's lower mantle (LM). This discussion explores the complex field of anharmonic effects due to phonon scatterings in MgO, specifically addressing their behavior under extreme high-pressure and high-temperature LM conditions. The objective is to determine the influence of these anharmonicities on lattice thermal conductivity. Conducting ab-initio analyses for two distinct scenarios: one simulating elevated temperatures up to 1223K and another replicating LM conditions with T-P values ranging from 1900K-24GPa to 3000K-130GPa. Our study employs Infrared and inelastic x-ray scattering observations performed in our team for benchmarking. A comparison with simulations validates joint Density Functional Perturbation Theory (DFPT) and self-consistent harmonic approximation (SSCHA) computations for vibrational energies and phonon lifetimes, ensuring theoretical predictions align with experimental data. Additionally, a simplified model is utilized to explore the impact of mass disorder on thermal conductivity. Descending into the lower mantle, our findings unveil an unexpected change in anharmonic properties, attributed to the interplay of extreme pressure and temperature.

MM 21.4 Tue 11:00 C 264

Strong Quartic Anharmonicity and Thermoelectric Performance in Antiperovskite — •Wenling Ren[1], Jincheng Yue[2], Shuyao Lin[1,3,4], Chen Shen[1], Yanhui Liu[2], Tian Cui[2], Harish Kumar Singh[1], Terumasa Tadano[5], and Hongbin Zhang[1] — [1]TU Darmstadt, Darmstadt, Germany — [2]Ningbo University, Ningbo, China — [3]TU Wien, Vienna, Austria — [4]Linkoping University, Linkoping, Sweden — [5]National Institute for Materials and Science, Tsukuba, Japan

Antiperovskite(APV) materials have garnered significant attention due to their rich physical properties. We employed a combination of SCP theory and the BTE, ultimately evaluating the thermal and electronic transport properties of APV (A_3XN,A=Mg,Ca,Sr;X=P,As,Sb,Bi). It is observed that such materials stand out for their strong quartic anharmonicity, stemming from the underlying exceptional lattice distortion. This leads to a relatively subdued temperature response concerning the lattice thermal conductivity, especially at elevated temperatures. Detailed analysis is done by investigating the dynamical stability and phonon scattering properties to elucidate the origin of reduced thermal conductivities. Further calculations on the electronic transport properties reveal that such materials exhibit promising thermoelectric figure of merit, i.e., up to 1.25, 1.03 and 1.03 for Ca_3BiN, Mg_3BiN and Sr_3BiN, respectively. Our work serves as a proof-of-concept example of a comprehensive exploration of APV materials, suggesting their significant potential for future medium/high-temperature thermoelectric applications.

MM 21.5 Tue 11:15 C 264

Role of anharmonicity in the lattice dynamics and thermal transport of different phases of $KNbO_3$ — •Niloofar Hadaeghi, Chen Shen, and Hongbin Zhang — Institute of Materials Science, Technical University of Darmstadt, Darmstadt, Germany

The $KNbO_3$ material, with its intriguing properties, has always been considered as a great (lead-free) candidate in the energy storage applications. However, despite the significant interest in its cubic, tetragonal, and orthorhombic phases, investigation of their lattice dynamics and lattice thermal transport have remained challenging, due the unstable phonon modes in the harmonic phonon dispersion bands. Here, utilizing self-consistent phonon theory and compressive sensing techniques, we explore the significant role of quartic anharmonicity in the renormalization of the harmonic interatomic force constants and hardening of the lattice modes in the temperature dependent phonon bands and density of states in the three phases. Moreover, the lattice thermal conductivity (LTC), along with the phonon lifetimes are studied for the three phases. The achieved results are in a good agreement with experimental values, where the lower experimental values are due to the higher different types of scattering related to the poly-crystalline nature in the experiment. For instance, the calculated result at 1000 K is 1.45 W/m.K for the cubic phase, where the experimental value is 1.2 W/m.K. The values of LTC at 300 K are as 4.2 W/m.K for the cubic, 7.3 W/m.K for the tetragonal and 7.8 W/m.K for the orthorhombic phases.