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S E M I N A R
on
Semiconductor Physics and Nanotechnology

Mo, 20.04.2026, 11:15 Uhr,

Seminar in
person in the physics lecture hall *or* via Zoom

"A quantitatively accurate understanding of thermal transport in complex materials in real and reciprocal space"

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Heat conduction is a crucial process for all applications in which excess heat needs to be either dissipated or supplied. In electrically insulating materials, the transport of thermal energy occurs via lattice vibrations, which can either be described in real space via the motion of atoms or in reciprocal space via the transport of quanta of vibrational energy (so-called phonons). To develop reliable structure-to-property relations for the thermal conductivity of complex materials, an atomistic understanding of the underlying processes is crucial. This understanding can be best achieved via atomistic computer simulations, provided that they are capable of providing a quantitatively accurate description of the relevant processes.

This raises two fundamental questions: which computational approach should be chosen to describe thermal transport, and how can one reliably describe the involved interatomic interactions? For the latter, density functional theory (DFT) would be the natural choice, but DFT is not efficient enough to calculate forces between (tens of) thousands of atoms several million times. At the other end of the computational spectrum would be classical, transferable force fields, but they are too inaccurate to provide a reliable description. This dilemma can be resolved using system-specifically machine-learned force fields, trained on DFT data. Here, this is implemented using so-called moment-tensor potentials trained via a specially adapted active learning approach.[1,2,6] This allows a quantitatively reliable description of heat transport processes, for example, in MOFs,[1] molecular crystals,[2] or crystalline polymers.[4] Quantitative agreement with accurate experiments (often on single crystals) is achieved both when extracting thermal conductivities from the particle trajectories of non-equilibrium molecular

dynamics simulations[1,4,5] and when basing the analysis on harmonic and anharmonic phonon properties.[3,4]

The distinct advantage of considering both real- and reciprocal-space approaches is that they provide complementary insight into the physical aspects of heat transport: from an analysis of the real-space effective temperature distribution in MOFs subject to a thermal gradient, one can, for example, identify local heat-transfer bottlenecks.[5,7] In contrast, analyzing the dynamics of phonons provides insight into the actual heat-transport mechanism, revealing that not only the particle-like motion of phonons, but also their tunneling becomes highly relevant in complex materials with low thermal conductivities.[3] Based on phonon properties, one can furthermore understand why in molecular crystals like naphthalene the thermal conductivity increases by about an order of magnitude at elevated pressures of ~2-3 GPa.[8]

[1] Sandro Wieser and Egbert Zojer, npj Comput. Mater. 2024, 10, 18; [2] Nina Strasser, Sandro Wieser, and Egbert Zojer, Int. J. Mol. Sci. 2024, 25, 3023; [3] Lukas Legenstein, Lukas Reicht, Sandro Wieser, Michele Simoncelli, Egbert Zojer, npj Comput. Mater. 2025, 11, 29.; [4] Lukas Reicht, Lukas Legenstein, Sandro Wieser, Egbert Zojer, npj Computational Materials (2026), published on-line; [5] Sandro Wieser, Tomas Kamencek, Johannes P. Dürholt, Rochus Schmid, Natalia Bedoya-Martínez, Egbert Zojer, Adv. Theory Simul. 2021, 4, 2000211; [6] Lukas Reicht, Lukas Legenstein, Sandro Wieser and Egbert Zojer, Molecules, 2024, 29, 3724; [7] Sandro Wieser, Tomas Kamencek, Rochus Schmid, Natalia Bedoya-Martínez, and Egbert Zojer, Nanomaterials 2022, 12, 2142; [8] Lukas Legenstein, Sandro Wieser, Michele Simoncelli, and Egbert Zojer, in preparation.

Zoom – Link:
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