Lehrstuhl für Physik

Department Physik, Mechanik und Elektrotechnik
Montanuniversität Leoben

A-8700 LEOBEN, Franz Josef Straße 18, Austria
Tel: +43 3842 402-4601
e-mail: physics@unileoben.ac.at

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

Mo, 15.12.2025, 11:15 Uhr,

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

"Modelling Heat Conduction in Crystalline Organic Semiconductors"

Dr. Lukas Legenstein

Chair of Physics, Department Physics, Mechanics and Electrical Engineering,
Technical University of Leoben, Austria

Understanding heat transport in organic semiconductors is crucial for improving their functionality. Therefore, the lattice thermal conductivities of prototypical acene crystals, where increasing molecular length introduces greater structural complexity, were modelled using machine-learned interatomic potentials. Experimental data reveal significant deviations from the traditionally-used Peierls–Boltzmann transport theory based on particle-like phonon transport. These discrepancies are resolved by including an additional conduction channel arising from phonon mode coupling, as formulated within the Wigner transport equation. This framework accounts for both the systematic increase in conductivity with molecular length and the glass-like temperature dependence observed in tetracene and pentacene crystals. Furthermore, the ability of the machine-learned potentials to describe these molecular crystals under high pressure was assessed, and improved models were employed to investigate the origins of pressure-induced changes in crystal structure and thermal conductivity.

Zoom – Link:
https://zoom.us/j/96375934537?pwd=RTlKTWhSdzRHU211YTY1bGFxTUtpZz09
Meeting-ID: 963 7593 4537
Kenncode: =r=4YQ