



清华大学高等研究院

Institute for Advanced Study, Tsinghua University

学术报告

Title: 2D thermoelectric materials: Role of the lattice thermal conductivity

Speaker: Udo Schwingenschlögl
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Abstract

We study the role of the lattice thermal conductivity in 2D thermoelectric materials by first-principles calculations. Specific examples include a comparison of Ti_2CO_2 , Zr_2CO_2 , and Hf_2CO_2 in order to evaluate the role of the metal atom. The lattice thermal conductivity is demonstrated to grow along the series Ti-Zr-Hf in the temperature range 300-700 K, resulting in the highest figure of merit in the case of Ti_2CO_2 . Flat conduction bands promote the thermopower in the case of n-doping. Functionalization effects are studied for Sc_2C , which is semiconducting for various functional groups, including O, F, and OH. The lowest lattice thermal conductivity is found for OH functionalization. Despite a relatively low thermopower, $\text{Sc}_2\text{C}(\text{OH})_2$ therefore and due to a high electrical conductivity can be interesting for intermediate-temperature thermoelectric applications. We also discuss results on heterostructures built of MXenes and transition metal dichalcogenide monolayers. Low frequency optical phonons are found to occur as a consequence of the van der Waals bonding. They contribute significantly to the thermal transport and compensate for reduced contributions of the acoustic phonons (strong scattering in heterostructures), such that the thermal conductivities become similar to those of the constituent MXenes.

Biography:

Dr. Schwingenschlögl is a Professor of Materials Science & Engineering at King Abdullah University of Science and Technology (KAUST). His research interests in condensed matter physics and first-principles materials modeling focus on two-dimensional materials, interface and defect physics, correlated materials, thermoelectric materials, metal-ion batteries, nanoparticles, and quantum transport. Dr. Schwingenschlögl joined KAUST as founding faculty member in 2008, having previously worked at the International Center of Condensed Matter Physics in Brasilia, Brazil, and the Universität Augsburg in Germany.