Modeling and Ab initio Calculations of Thermal Transport in Si-Based Clathrates and Solar Perovskites
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We present calculations of the thermal transport coefficients of Si-based clathrates [1,2] and solar perovskites [3], as obtained from ab initio calculations and models, where all input parameters derived from first principles. We elucidated the physical mechanisms responsible for the measured low thermal conductivity in Si-based clathrates [1] and predicted their electronic properties and mobilities, which were later confirmed experimentally [2]. We also predicted that by appropriately tuning the carrier concentration, the thermoelectric figure of merit of Sn and Pb based perovskites may reach values ranging between 1 and 2, which could possibly be further increased by optimizing the lattice thermal conductivity through engineering perovskite superlattices.


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