Thermal Conductivity Modeling for Hybrid Materials: from Density Functional Theory to Molecular Dynamics

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There have been increasing interests in hybrid inorganic-organic materials, which could combine the strengths of both components, for example, good electronic properties from inorganic part and superb flexibility and easiness in synthesis from organic part. Unlike the electronic and mechanical properties, the thermal properties of hybrid materials are rarely investigated. Understanding thermal properties of the hybrid materials is critical for the deployment of these materials for electronics and optoelectronics since it affects the reliability. In addition, hybrid materials could be explored for potential applications in thermal management and storage. In this project, $ZnTe(en)_{0.5}$, a layered hybrid crystal whose organic chain and inorganic layers are connected by covalent bonds, will be chosen as a first attempt to understand the thermal transport mechanisms in the class II hybrid materials. Such a hybrid crystal with covalent bonding could exhibit quite different thermal transport properties from class I hybrid materials with weak bonding, such as van der Waals or hydrogen bonding. An integrated density-functional theory (DFT) and molecular dynamics (MD) simulation tool will be developed to study the phonon transport properties in $ZnTe(en)_{0.5}$, where the interatomic potentials is developed by fitting a series of properties of $ZnTe(en)_{0.5}$ calculated from DFT calculations and the MD simulations is then conducted to predict its thermal conductivity.