Understanding thermal transport in Transition Metal Dichalcogenides: from the monolayer to the bulk

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Layered Transition Metal Dichalcogenides (TMDs) have received significant attention in the past years because of their exceptional properties, which differ from those of 3D-bonded materials. Reaching an understanding of their thermal properties is crucial for many applications e.g., in electronics and thermoelectrics. We present a theoretical study of the phonon heat transport properties of WS_2, WSe_2, MoS_2 and $MoSe_2$, from the monolayer to the bulk. We calculate the thermal conductivity of TMDs by solving the Boltzmann Transport Equation for phonons, using input from first principles calculations. We use the SIESTA method, based on Density Functional Theory, to compute ab-initio energies and forces from which we obtain the phonon structure and the phonon-phonon interactions using the Temperature Dependent Effective Potential package for finite temperature lattice dynamics calculations. We compute the thermal properties for the TMDs at room temperature and compare the results with experiments on a full range of thicknesses, which demonstrates the reliability and efficiency of our computational method [3]. We compare the results for different TMDs and reach a unifying picture of heat transport in 2D-bonded semiconductors, which will be useful for future technologies.

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References

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Figures

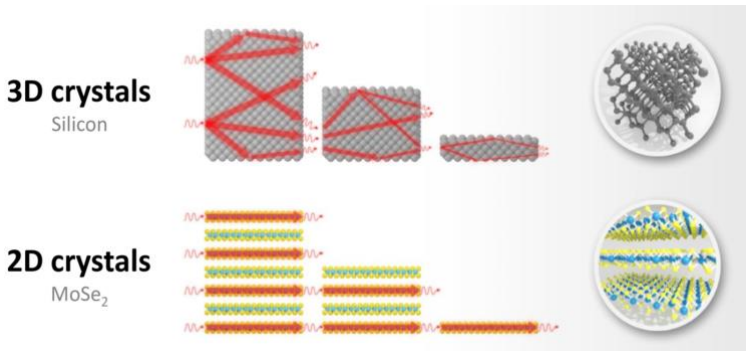

Figure 1: Schematic view of the heat transport mechanism in 3D materials compared to layered materials composed of 2D sheets. In the latter case, thermal conductivity is quite unsensitive to the thickness, as heat is transported within each layer.