Understanding thermal transport in 2D Transition Metal Dichalcogenides

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Layered Transition Metal Dichalcogenides (TMDs) have garnered considerable attention in recent years due to their remarkable characteristics, which differ from those of 3D-bonded material. Gaining insight into their thermal properties is of utmost importance for various applications, such as electronics and thermoelectrics [1]. In this study, we present a theoretical investigation focused on the heat transport properties of WS_2, WSe_2, MoS_2, and $MoSe_2$, in monolayer and bulk configurations. By solving the Boltzmann Transport Equation for phonons and utilizing inputs derived from first principles calculations, we determine the thermal conductivity of those TMDs. To obtain the phonon structure and phonon-phonon interactions, we employ the SIESTA method [2,3], based on Density Functional Theory, and utilize the Temperature Dependent Effective Potential package for lattice dynamics calculations at finite temperatures [4]. We compare the obtained thermal properties with experimental data, demonstrating the reliability and efficiency of our computational approach [5]. By comparing the outcomes for different TMDs, we arrive at a comprehensive understanding of heat transport in 2D-bonded semiconductors, offering valuable insights for future technological advancements.

References

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