Thermal Transport Properties of 2-Dimensional Transition Metal Dichalcogenide Heterostructures

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Manipulating heat is an ancient art that sparked human civilization and continues to attract significant interest from the scientific community. Materials with low thermal conductivities can be used to effectively control heat. Two-dimensional (2D) transition metal dichalcogenides (TMDs) such as WSe2 are known to exhibit thermal conductivities as low as 0.05W/mK. In this work, I systematically investigated a series of 2D TMDs using large scale molecular dynamics simulations, confirming the experimentally reported thermal conductivity of WSe2 and MoS2. Furthermore, I revealed that MoSe2 exhibits an even lower thermal conductivity of 0.022W/mK, and I discovered that WSe2-MoSe2 heterostructure has a groundbreaking thermal conductivity of 0.0096W/mK, lower than both of its constituents and, in fact, any known solids. Preliminary experimental testing has also been carried out to measure the thermal conductivities of 2D TMDs. If confirmed, the ultralow thermal conductivity of the WSe2-MoSe2 heterostructure may find many applications in thermal management.

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