

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.

Awards Won:

Air Force Research Laboratory on behalf of the United States Air Force: First Award of \$750 in each Intel ISEF Category