Heat Transport in Transition Metal Dichalcogenides from first principles calculations

Roberta Farris[1]
D. Saleta Reig[1], S. Varghese[1], A. Block[1], O.Hellman[2], K. J. Tielrooij[1], P. Ordejón[1], Z. Zanolli[3], M. J. Verstraete[4]

[1]*Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and BIST, Campus UAB, Bellaterra, 08193, Barcelona, Spain*
[2] Departament of Molecular Chemistry and Materials Science, *Weizmann Institute of Science, Rehovot 76100, Israel*
[3]*Chemistry Department & Debye Institute for Nanomaterials Science, Utrecht University, the Netherlands*
[4]*Université de Liège, Département de Physique, B-4000 Sart Tilman, Liège, Belgium*
roberta.farris@icn2.cat

Layered 2D Transition Metal Dichalcogenides (TMDs) have received significant attention because of their unique electrical, optical, and mechanical properties that may be in contrast with those of their bulk parent compounds. In contrast, thermal properties and how they change from a 3D crystal to a 2D layered structure have received less attention even though their understanding is crucial for several applications exploiting these materials, such as thermoelectricity and optoelectronics [1].
Here, we present a theoretical study of the intrinsic lattice thermal conductivity of bulk and monolayer WS_2, WSe_2, MoS_2 and $MoSe_2$ focusing on the dependence of heat transport on the atomic mass and atomic species present in the compounds.
This study allows us to understand the role of the different atomic species involved in the thermal transport when we pass from a 3D structure to a 2D structure and the implications at the microscopic level, including a complete inverstigation of the scattering rates and phonon frequencies.
The thermal conductivity κ of TMDs is calculated by solving the Boltzmann Transport Equation (BTE) including phonon-phonon scattering and phonon boundary scattering beyond the relaxation time approximation (RTA) [2].
First principles calculations are accurately performed by the SIESTA program [3] based on the Density Functional Theory (DFT) and the Temperature Dependent Effective Potential package (TDEP) [4] for finite temperature lattice dynamics calculations.
By employing this method we computed the thermal properties for the different TMDs at room temperature and we compare the results with recent and accurate experiments on a full range of thicknesses [5].

References

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