

Thermal transport modelling through van der Waals heterostructures

Sara Fiore

Mathieu Luisier

Integrated Systems Laboratory, ETH Zürich, 8092 Zürich, Switzerland

safiore@iis.ee.ethz.ch

Abstract

We have developed an advanced modelling approach to shed light on the thermal transport properties of van der Waals heterostructures (vdWHs) composed of single-layer transition metal dichalcogenides (TMDs) stacked on top of each other with a partial overlap region in the middle [1],[2]. Better understanding their thermal flow might be critical to design future, vdWH-based components with either well-controlled heat dissipation or high thermoelectric conversion efficiency. Here, we focus on ballistic quantum transport (QT) simulations of phonons through the vdWHs depicted in Fig. 1. The required dynamical matrices are first computed via density functional theory (DFT) and then passed to a QT tool relying on the Non-equilibrium Green's Function formalism to perform transport calculations. A temperature gradient is applied between both structure extremities, enabling a thermal current to propagate from the hot to the cold contact. Microscopically, vibrations are transferred from one layer to the other along the overlap region. The latter acts as a filter selecting out the states that can pass through it and modulating the amount of heat transferred according to its length, in a similar way as a resonant cavity. The injected waves build constructive and destructive interferences whose properties depend on the TMD choice and on the vdWH geometry, as illustrated in Fig. 2. Hence, our work emphasizes the possibility of engineering nanoscale heat flows by combining TMD monolayers.

References

- [1] "Two-dimensional van der Waals materials", P. Ajayan, K. Banerjee, *Physics Today*, 9(2016), 38.
- [2] "Van der Waals heterostructures", Geim, A. K., Grigorieva, I. V., *Nature*, 2013.

Figures

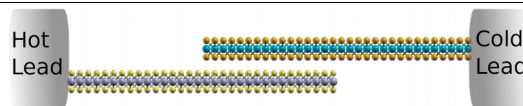


Figure 1: van der Waals device configuration with two TMD monolayers partially overlapping.

