Phononics in two-dimensional materials

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Over the last years, two-dimensional (2D) materials have attracted considerable interest due to the fact that they offer a new broad playground to explore and develop nanoscale devices with tailored electrical, optical and thermal properties [1]. Recently, many prototypes have been proposed for thermal devices (diodes, transistors, and logic gates) based on graphene [2]. Most of these investigations have focused on how to control the heat flux in order to display heat rectification. Moreover, from the point of view of simulating heat transport, it has been shown a great improvement in the development of advanced computational methodologies in order to gain a deep insight into the mechanisms governing thermal transport properties in nanomaterials[3, 4].

Hence, in the present work, we use non-equilibrium molecular dynamics (NEMD) simulations to study the thermal rectification effect in asymmetric MoS_2 and hBN-C nanoribbons. We show that thermal rectification ratios of up to 25 % can be achieved in dependence of the asymmetry degree of the ribbons. It has also been proved that this effect can be tuned by surface engineering. Also, we combine non-equilibrium Green's functions (NEGF) technique with a density functional tight-binding (DFTB) approach to study the influence of diverse factors on the thermal transport properties of novel 2D materials. In the ballistic phonon transport regime, we have found out that the effect of ad-atoms and molecular functionalization on the thermal properties of graphene grain boundaries (GBs) sensitively depends on their structural configuration. Anisotropic thermoelectric properties have been also found in two-dimensional puckered structures. Thermal transport properties have also been tuned by strain engineering in hBN, phosphorene, MoS_2 monolayers, and their corresponding 4|8 and 5|7 grain boundaries.

References

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Figures

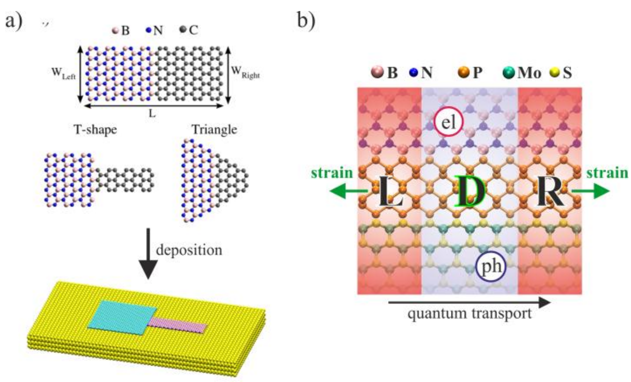

Figure 1. a) Scheme of the deposition on a substrate of thermal diode prototypes made of hBN-C nanoribbons. b) Transport setup for computing thermal transport properties by using NEGF technique.