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POSTER No. 1

Anistoropic Phononic Thermal Conductivity of Arsenene: An *ab initio* Study

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Abstract:

Elemental 2D materials exhibit intriguing heat transport and phononic properties. Here we have investigated the lattice thermal conductivity of newly proposed arsenene, the 2D honeycomb structure of arsenic, using *ab initio* calculations. Solving the Boltzmann transport equation for phonons, we predict a highly anisotropic thermal conductivity, of 30.4 and 7.8 W/mK along the zigzag and armchair directions, respectively at room temperature. Our calculations reveal that phonons with mean free paths between 20 nm and 1 μm provide the main contribution to the large thermal conductivity in the zig-zag direction, mean free paths of phonons contributing to heat transport in the armchair directions range between 20 and 100 nm. The obtained low and anisotropic thermal conductivity, and feasibility of synthesis, in addition to other reports on high electron mobility, make arsenene a promising material for a variety of applications, including thermal management and thermoelectric devices.

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POSTER No. 2

Thermal Rectification in Asymmetric Nanostructures: Molecular Dynamics Studies

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Abstract:
Recent progresses in manufacturing nanoscale electrical and mechanical devices have motivated deep understanding of heat transport in low dimensional systems and introducing new mechanisms for heat managements. More interestingly, it has been shown that thermal transport in many cases, e.g. carbon based nanostructures, are phonon dominated, indicating that phonons can be manipulated similarly to electrons for controlling heat transport at all temperatures [1]. Thermal rectification, the thermal counterpart of electrical diodes corresponding a better thermal conductance in one direction rather than the opposite one, can also play an important role in nanoscale heat management [2,3]. Here, we will try to briefly give an overview on our recent results, by utilizing molecular dynamics simulation, on studying thermal transport in low dimensional systems. Our recent results on phononic heat transport in low dimensional systems, in particular, the anisotropy importance and/or the effect of functionalization on thermal rectification in graphene [4,5], carbon nanotubes [6, 7] and silicene [8], will be discussed.

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