ARL/Master Thesis

in the group of *Theory of Magnetic Materials* (FB11)

TECHNISCHE UNIVERSITÄT DARMSTADT

Designing Thermal Management Materials

Both three-dimensional and two-dimensional materials with high (better tunable) thermal conductivities are critical for engineering the next-generation of electronic devices. However, how to evaluate the thermal conductivities and thus predict thermal management materials is still a challenging task. In my group, we have applied the recently developed compressive sensing technique based on machine learning to perform reliable calculations on the anharmonic effect (i.e., phonon-phonon interaction) and thus the thermal conductivities.

In this project, we are going to perform massive density functional theory calculations to evaluate the thermal conductivities for both 2D and 3D insulators with large band gaps, with a particular focus on those cases with tunable structural phase transitions. If time allows, we will also carry out explorative calculations to get the interfacial thermal resistance. Such activities will be guided by experienced PhD students in the group, thus publication(s) is expected.

For the motivated candidates, expertise will be gained on parallel computation, coding with Python, and compressive sensing, and solid experience on sophisticated density functional theory calculations, valuable for both future PhD studies and industrial positions.

Please write Prof. Hongbin Zhang (Email: hongbin.zhang@tu-darmstadt.de) if you are interested.

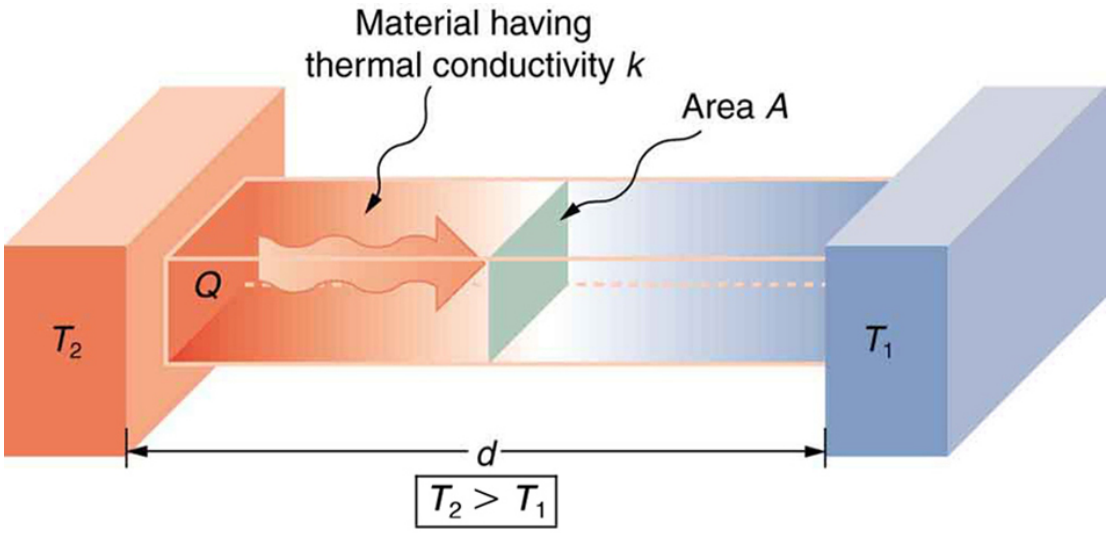

FIG. 1: Sketch of thermal conductivity driven by temperature gradients.