Comprehensive Atomistic Modeling of Thermoelectric Semiconductor Nanowire Heterostructures

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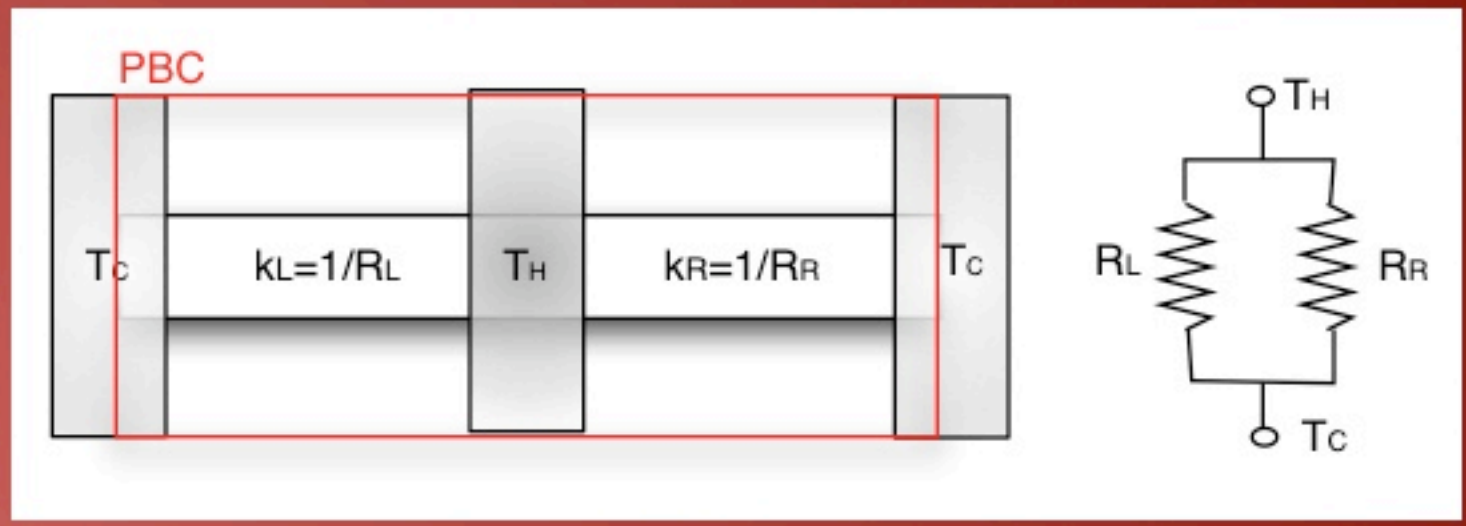
***Thermal Conductivity**: The efficiency of thermoelectric devices in converting heat into electrical work is inversely proportional to the thermal conductivity of the material. By using an analogy between heat and electricity, we have devised a method for computing the directional dependence of thermal conductivity, while avoiding finite size effects in our simulation and conserving energy. Calculations are now under way reporting the thermal conductivity and anisotropy of the primitive defects in wurtzite nanowires.*



Our study of thermoelectrics has also resulted in two spin-off projects:
(1) The simple pi-electron model used to develop and test our thermoelectric calculations was subsequently used to study multiple exciton generation in graphene nanostructures*; this study identified optimal structures that can* lead to a 30-80% increase in photocurrent. *(2) The thermoelectric effect can be more generally understood in terms of electrochemical potentials; instead of producing electrical work, one can use temperature gradients to produce "separation" work (i.e., Gibbs energy of mixing). This requires energy-selective particle transmission, which is most easily achieved using quantum mechanical effects. Based on this insight, we studied the feasibility of using an existing, chemically-synthesized* porous graphene membrane to separate Helium from natural gas*, and have demonstrated the role of quantum mechanical tunneling in the transmission of Helium atoms. These structures can be used to perform a "thermoelectrochemical" separation of ^{3}He from ^{4}He using the mass dependence of quantum mechanical tunneling.*