Comprehensive Atomistic Modeling of Thermoelectric Semiconductor Nanowire Heterostructures

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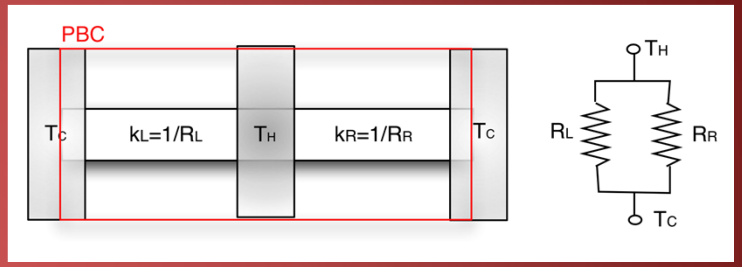
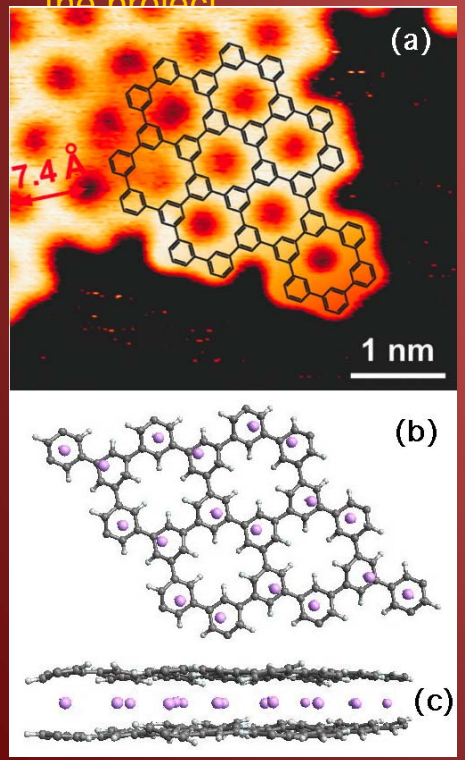
The additional thermal resistivity introduced by zinc-blende/wurtzite stacking faults in nanowires is smaller than the typical statistical error in a molecular dynamics simulation. Therefore, we conclude that introducing these types of defects into nanowires is not useful for increasing the thermoelectric figure of merit, *ZT*, which we hypothesized at the beginning of the project.





Moving forward, we intend to use the same methodologies developed in this project (reverse-non-equilibrium molecular strategy for calculating the thermal conductivities, followed by use VASP and BoltzTrap to compute the electronic terms in *ZT*), to study lithiated-porous graphene structures, which we hypothesize to have high-*ZT* due to:

- Low thermal conductivity, due to bond strength mismatch differences between intra-plane and inter-plane bonding (analogous to layered WSe_2)
- Narrow band gap semiconductor, with preliminary DFT calculations indicate 0.050 eV direct gap (underestimated by DFT, optimum for thermoelectric is 6-10 k_BT)
- Sharp peaks in electronic density of states due to Li-benzene interactions