Magnetic and Organic Nanowires to Enhance the Thermoelectric Figure of Merit via Electron/Phonon Transport Studies

磁性與有機導電奈米線提升熱電優值之電聲子傳播研究

Department of Power Mechanical Engineering, National Tsing Hua University

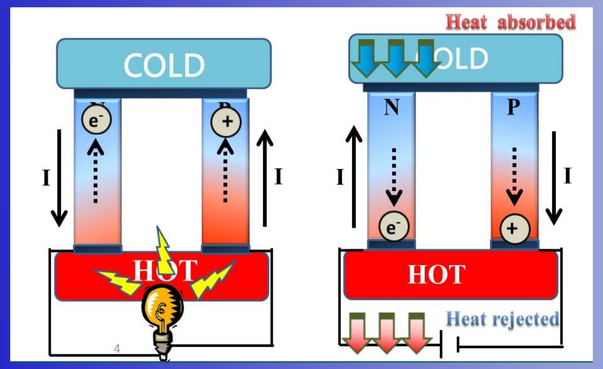
Chun-Ju Huang(黃俊儒) (Research student), Che-Wun Hong (洪哲文) (Professor)

Green Energy & Molecular Engineering Lab

◆Objective

1. To investigate the electrical and thermal properties of Si/SiGe nanowires, with/without magnetic effect, and PEDOT nanowires by first principles calculations.
2. To calculate and compare the thermoelectric properties between various nanowires, by using the Boltzmann transport equation. And also to find out the maximum ZT value by altering carrier concentrations.

◆Thermoelectric Generator and Thermoelectric Cooler



◆1D Boltzmann Transport equation

$$\frac{\partial f}{\partial t}+\vec{v}\cdot\nabla f+q\vec{E}\cdot\frac{\partial f}{\partial \vec{p}}=\frac{f_0-f}{\tau}$$

$$C_v(T)=k_B\int\frac{\left(\frac{\hbar\omega}{kT}\right)\exp\left(\frac{\hbar\omega}{kT}\right)}{\left[\exp\left(\frac{\hbar\omega}{kT}\right)-1\right]^2}D(\omega)\,\mathrm{d}\omega$$

$$V_g=d\omega/dk$$

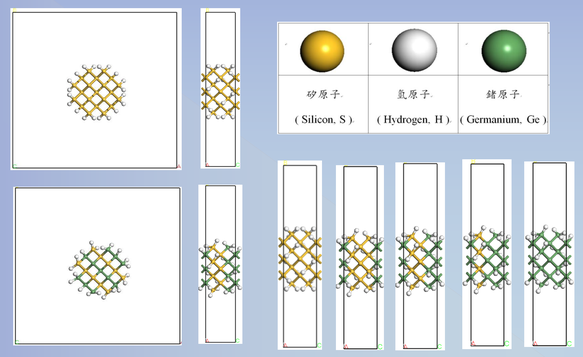
$$k_{ph}=\frac{1}{3}C_{ph}V_g l=\frac{1}{3}C_{ph}V_g^2\tau$$

$$\sigma\equiv\frac{J_z}{E_z}=\left(-\frac{2q^2}{3m}\int_{E=0}^{\infty}\frac{\partial f_0}{\partial E}D(E)E\tau dE\right)$$

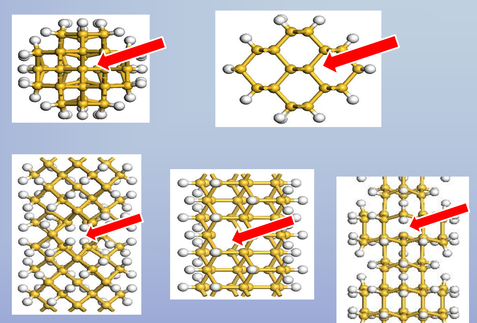
$$S=-\frac{1}{qT}\left(\mu-\frac{\int_{E=0}^{\infty}\frac{\partial f_0}{\partial E}D(E)E^2\tau dE}{\int_{E=0}^{\infty}\frac{\partial f_0}{\partial E}D(E)E\tau dE}\right)$$

$$k_e=\frac{2}{3mT}\left(\frac{\left(\int_{E=0}^{\infty}\frac{\partial f_0}{\partial E}D(E)E^2\tau dE\right)^2}{\int_{E=0}^{\infty}\frac{\partial f_0}{\partial E}D(E)E\tau dE}-\int_{E=0}^{\infty}\frac{\partial f_0}{\partial E}D(E)E^3\tau dE\right)$$

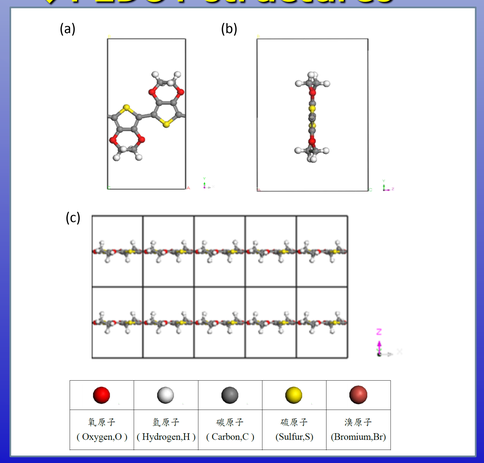
◆SiGeNWs structures



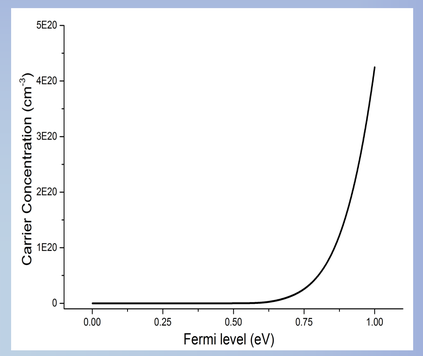
◆Defect Si structures



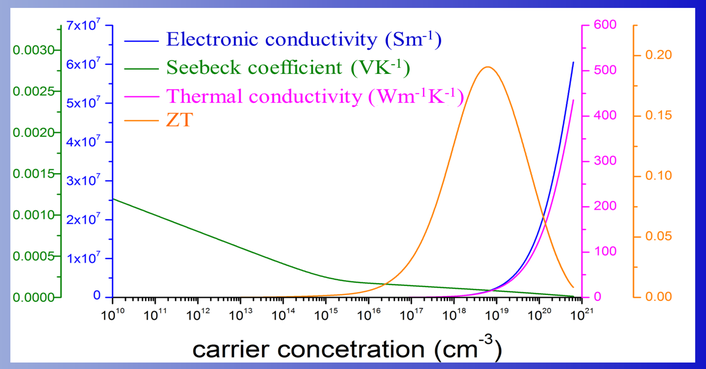
◆PEDOT structures



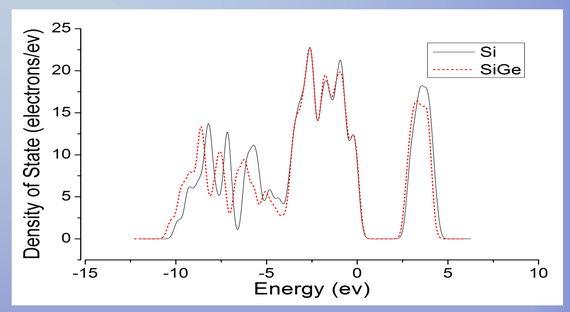
◆Fermi level and Carrier Concentration



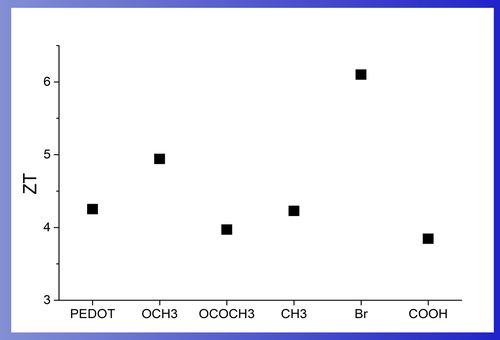
◆Thermoelectric parameter and Carrier concentration



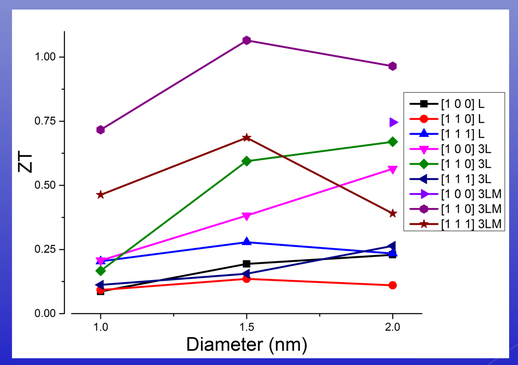
◆SiGe NWs DOS



◆PEDOT NWs ZT



Magnetic Si NWs ZT



All ZT Comparison