ID: P1.6

Title: Surface nitrogenation tuning the thermal conductivity of silicon nanowires: a molecular dynamics study

Name: Li, Haipeng

Affiliation: Department of Physics and Materials Science, City University of Hong Kong, Hong Kong SAR, People?s Republic of China.

Silicon nanowires (SiNWs) have been attracting great attention as promising building blocks for nanoelectronic devices as well as thermoelectric devices where a minimal thermal conductivity is required to convert heat into electricity directly. A better understanding of heat transport in SiNWs is highly desirable for silicon based nanoelectronic and thermoelectric applications. As already known, due to the large surface to volume ratio, the surface atoms have an important influence on the overall electronic properties for SiNWs. Besides the electronic properties, thermal conductivity is expected to be sensitive to surface functionalization of SiNWs. However, very little efforts have been directed to the thermal conductivity of surface passivated SiNWs. In this work, we have investigated the thermal conductivity of surface nitrogenated thin SiNWs using equilibrium molecular dynamics simulations. We have shown that surface nitrogen passivation can significantly reduce the thermal conductivity of SiNWs. The reduction in the thermal conductivity arises from the decrease of phonon mean free path and the suppression of some lattice vibrational modes due to surface nitrogenation. Our simulation results clearly demonstrate the importance of surface functionalization in tuning the thermal conductivity, which has profound implications for thermoelectric applications of SiNWs.