

First-Principles Simulations of Inorganic Nanowires

Junwen Li, Thushari Jayasekera, and John W. Mintmire

Department of Physics, Oklahoma State University, Stillwater, OK 74078

We report first-principles simulation results for the electronic band structure of silicon nanowires along the $\langle 100 \rangle$ and $\langle 110 \rangle$ directions using an all-electron Gaussian orbital local-density functional approach. We have examined the effects on the electronic structure of different chemical groups, such as hydrogen, hydroxyl, and methyl units, serving to passivate the nanowire surface. We discuss how the presence of these different substituents providing surface passivation affects the band gaps and electron distributions of silicon nanowires. Examining the band structures we find that the carrier effective masses of the $\langle 100 \rangle$ -oriented silicon nanowires exhibit a stronger dependence on the diameter and surface substituents than do the $\langle 110 \rangle$ -oriented nanowires. We have also carried out preliminary calculations on electron transport properties of the nanowires using a Landauer-Büttiker approach. In particular, we have examined the effect on electron transport of a small defect region in a silicon nanowire with different surface passivation that connects two silicon nanowire leads with hydrogen passivation.

This work is supported by the US Department of Energy Grant DE-FG02-07ER46362.