Ab initio computations of structural and electronic properties of doped and undoped Ge nanowires

D. MEDABOINA, V. GADE, Department of EECS, S. K. R. PATIL, Department of MIME, S. V. KHARE1, Department of Physics, University of Toledo, OH 43606 — We report results of structural and electronic properties of hydrogen passivated doped and undoped Ge nanowires along [100], [110] and [111] growth directions using density functional theory in the local density approximation (LDA). Cross-sections of nanowires with diameters \( d > 2.0 \text{ nm} \) are faceted reflecting the crystal symmetry about their axis. Nanowires along [100] direction with \( d \) below (above) 1.5 nm are found to be direct (indirect) band gap (\( E_g \)) semiconductors. Nanowires along [110] have direct \( E_g \) for \( d > 1.0 \text{ nm} \). Nanowires along [111] have indirect \( E_g \) for \( d > 1.0 \text{ nm} \). The magnitude of \( E_g \) increases as the wire diameter decreases with values as high as 4.3 eV for a [100] wire with \( d = 0.41 \text{ nm} \). For a fixed diameter \( E_g^{[100]} > E_g^{[111]} > E_g^{[110]} \). Doping with P or B did not have a significant effect on the valence and conduction band dispersions.

1Correspondence: khare@physics.utoledo.edu

Sanjay Khare
Department of Physics, University of Toledo

Date submitted: 20 Nov 2006  Electronic form version 1.4