Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

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. KHARE[1], 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 nm are facetted 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 nm. Nanowires along [111] have indirect E_g for d > 1.0 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 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.

[1]Correspondence: khare@physics.utoledo.edu

Sanjay Khare
Department of Physics, University of Toledo

Date submitted: 20 Nov 2006 Electronic form version 1.4