

Electronic Structure of Core-Shell Semiconductor Nanowires

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(Dated: June 5, 2006)

We investigate the electronic structure of silicon/germanium core-shell nanowires with first-principles calculations using the local density approximation (LDA) with pseudopotentials and plane waves. The atomic configurations of the core-shell nanowires are fully relaxed. By examining the wave functions in real space, the electronic states at the band edge are found to be confined in either the core or the shell part of the nanowire. The band offsets are calculated for different core-shell structures. Given the cylindrical band offsets and the associated confined electronic states, a novel doping mechanism in nanowires is proposed for the manufacturing of high-speed nano-devices.

PACS numbers: Valid PACS appear here