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Electronic Structure of Core-Shell Semiconductor Nanowires LI YANG, MEI-YIN CHOU, Georgia Institute of Technology — 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 localized 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.

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