Electronic Structure of Core-Shell Semiconductor Nanowires LI
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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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