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First principles study of strained Si/Ge core-shell nanowires along [110] direction XIHONG PENG, PAUL LOGAN, Arizona State University — First principles density-functional calculations were performed to study the electronic properties of Si/Ge core-shell nanowires along the [110] direction with the diameter of the wires up to 5 nm. It was found the band gap of the core-shell wires is smaller than that of both pure Si and Ge wires, given the same diameter. This reduced band gap is ascribed to the intrinsic strain between Ge and Si layers, which partially counters the quantum confinement effect. External uniaxial strain is further applied to the Si/Ge core-shell nanowires for tuning the band structure. At the Γ point, the energy levels of both conduction and valence bands are significantly altered by applied strain, which results in an evident change of the band gap. In contrast, for the K vectors far away from Γ, the variation of the conduction/valence band with strain is much reduced. In addition, with a sufficient tensile strain ($\sim$1%), the valence band edge shifts away from Γ, which indicates that the band gap of the Si/Ge core-shell nanowires experiences a transition from direct to indirect.

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