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Quantum Confinement in Strained Si/Ge Core-Shell Nanowires

PAUL LOGAN, XIHONG PENG, Arizona State University — First principle calculations based on density-functional theory were performed to study quantum confinement on the electronic properties of strained Si/Ge core-shell nanowires along the [110] direction with the diameter up to 5 nm. Particularly the band gap and the effective masses of the electron and hole were investigated. As shown in the calculations, the Si/Ge core-shell [110] nanowires possess a direct band gap, in contrast to the nature of an indirect band gap in bulk Si and Ge. The band gap of the core-shell wires is decreased compared with the pure Si or Ge nanowires with the same size. This reduced gap is ascribed to the intrinsic strain in the core-shell wires, which partially counters the quantum confinement effect. Moreover, the effects of unaxial strain on the effective mass and hole will be discussed.

Paul Logan
Arizona State University

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