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The Effects of Strain and Quantum Confinement on the Electronic Properties of Germanium Nanowires[1] PAUL LOGAN, Arizona State Univeristy, XIHONG PENG, Arizona State University — Germanium nanowires are expected to play an important role as both interconnects and functional components in future nanoscale electronic and optical devices, such as light-emitting diodes, field-effect transistors, chemical and biological sensors. The study of quantum confinement on the band gap of Ge nanowires have been addressed both using theoretical methods and experimental techniques. In the present work, using first principles density-functional theory we studied the uniaxial strain effects on the electronic properties in Ge wires along [110] direction with lateral diameter up to 5 nm. Ge [110] nanowires demonstrate a direct band gap, in contrast to the nature of indirect band gap in bulk. We discovered that the uniaxial strain modulates the band gap of Ge nanowires: compressive strain increases the gap while tensile strain reduces the gap. In addition, the strain also modifies the effective masses of the electron and the hole of Ge wires. Expansion increases the effective mass of the hole, while compression increases the effective mass of the electron. Our results suggest both strain and size can be used to tune the band structure of nanowires, which may help in design of future nanoelectronical devices.

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