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Electronic Properties of Strained Si [111] Nanowires PAUL LOGAN, XIHONG PENG, Arizona State University — First principles density-functional theory was used to calculate the effects of strain on the electronic properties of Si nanowires along the [111] direction for wires up to 2.5 nm in diameter. Our results show that the Si [111] nanowires can have direct or indirect band gaps depending on the amount of strain applied to the wires. The exact strain required for the transition from indirect to direct gap was thoroughly investigated in nanowires with different diameters. The larger the nanowire, the larger expansive strain is required to produce a direct band gap. In addition, our calculations reveal a strong dependence of both the gap and effective masses of electrons and holes on the applied strain. We discussed our results in terms of bonding/antibonding and orientation of the electron orbitals near the conduction and valence band edges.

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