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Confinement of electrons in size modulated silicon nanowires SEYMUR CAHANGIROV, SALIM CIRACI[1], UNAM-Institute of Materials Science and Nanotechnology, Bilkent University, Ankara 06800, Turkey, CIRACI GROUP TEAM — Based on first-principles calculations we showed that superlattices of periodically repeated junctions of hydrogen saturated silicon nanowire segments having different lengths and diameters form multiple quantum well structures. The band gap of the superlattice is modulated in real space as its diameter does and results in a band gap in momentum space which is different from constituent nanowires. Specific electronic states can be confined in either narrow or wide regions of superlattice. The type of the band lineup and hence the offsets of valence and conduction bands depend on the orientation of the superlattice as well as on the diameters of the constituent segments. Effects of the SiH vacancy and substitutional impurities on the electronic and magnetic properties have been investigated by carrying out spin-polarized calculations. Substitutional impurities with localized states near band edges can make modulation doping possible. Stability of the superlattice structure was examined by ab initio molecular dynamics calculations at high temperatures.

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