

Abstract Submitted
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First Principles Studies of the Structural and Opto-Electronic Properties of Silicon Nanowires¹ TRINH VO, LLNL, ANDREW WILLIAMSON, LLNL, GIULIA GALLI, UC Davis and LLNL — We report the results of first principles studies of the structural, electronic, and optical properties of hydrogen-passivated silicon nanowires with [001], [011], and [111] growth directions and diameters ranging from 1 to 3 nm. We show that the growth direction, diameter, and surface structure all have a significant effect on the structural stability, electronic band gap, band structure, and band edge effective masses of the nanowires. The band gap is found to decrease with increasing diameter and to be further reduced by surface reconstruction. The band gap is direct for [001] and [011] NWs with diameters smaller than 3nm and [111] NWs with diameters smaller than 2nm. While the electron and hole effective masses are found to depend on NW size for [001] and [111] NWs, they are almost independent of size for [011] NWs. Finally, we use FEFF calculations to predict the EXAFS spectra produced by the relaxed atomic structure of the NWs and show that these spectra can serve as a tool for detection of surface reconstructions of the NWs.

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