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Electronic structure calculations of tapered silicon nanowires ZHIGANG WU, SHAN-HAW CHIOU, University of California, Berkeley , JEFFREY NEATON, Lawrence Berkeley National Lab, JEFFREY GROSSMAN, University of California, Berkeley — Nanowires are observed experimentally to be tapered rather than straight-edged, with diameters shrinking by as much as 1 angstrom per every 10 angstroms of vertical growth, depending on the synthesis technique and conditions. Yet, most theoretical work to understand the electronic, optical, and structural properties of nanowires have assumed a straight-edge geometry. In this work, we focus on the impact of tapering on nanowire properties. Using ab initio pseudopotential calculations, we show that tapered silicon nanowires have axial-dependent electronic structure properties due to quantum confinement effects. Other electronic and structural properties related to the tapering will also be presented. Further, we illustrate how these properties may be advantageous for nanowire- based photovoltaic applications, where the highest absorption efficiency and lowest thermalization loss for a photon occurs when it has an energy close to the gap of the solar cell.

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