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First Principles Studies of Tapered Silicon Nanowires: Fundamental Insights and Practical Applications

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Nanowires (NWs) are often observed experimentally to be tapered rather than straight-edged, with diameters (d) shrinking by as much as 1 nm per 10 nm of vertical growth. Previous theoretical studies have examined the electronic properties of straight-edged nanowires (SNWs), although the effects of tapering on quantum confinement may be of both fundamental and practical importance. We have employed ab initio calculations to study the structural and electronic properties of tapered Si NWs. As one may expect, tapered nanowires (TNWs) possess axially-dependent electronic properties; their local energy gaps vary along the wire axis, with the largest gap occurring at the narrowest point of the wire. In contrast to SNWs, where confinement tends to shift valence bands more than conduction bands away from the bulk gap, the unoccupied states in TNWs are much more sensitive to d than the occupied states. In addition, tapering causes the band-edge states to be spatially separated along the wire axis, a consequence of the interplay between a strong variation in quantum confinement strength with diameter and the tapering-induced charge transfer. This property may be exploited in electronic and optical applications, for example, in photovoltaic devices where the separation of the valence and conduction band states could be used to transport excited charges during the thermalization process. In order to gain insight into TNW photovoltaic properties, we have also carried out calculations of the dipole matrix elements near the band edges as well as the role of metal contacts on TNW electronic properties. Finally, a combination of ab initio total energy calculations and classical molecular dynamics (MD) simulations are employed to suggest a new technique for bringing nanoscale objects together to form ordered, ultra high-aspect ratio nanowires. This work was supported in part by the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.