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Electronic structures and optical properties of silicon nanowires
JUN LI, Northwestern University, ARTHUR FREEMAN — Recent optical spectroscopic[1] and theoretical/computational studies[2] challenge the previous consensus on the nature of the optical properties of Si nanowires (SiNW). Here, we present results of precise theoretical FLAPW [3] determinations of the electronic structures and optical properties of (001) and (111) one nm SiNW. The electronic states at the gaps demonstrate a strong orientation dependent parabolic character in the Brillouin zone and a clear entanglement in real space between 1D and 2D dimensions of the wire. The local symmetry imposed by quantum confinement quenches the transitions around the gap, yielding an optically inactive direct gap. The observed (001) photoluminescence is attributed to a transition rooted in an Si_8 ring. The optical structure in the experimental range is well reproduced by our first-principles calculations that include the screened exchange-LDA correction to the well-known failure of the LDA. Our predictions about the anisotropy and orientation dependent optical absorption are easily verified experimentally. Work supported by DARPA B529527//W-7405-Eng-48.

[1]Holmes, Johnston, Doty, and Korgel, Science 287, 1471 (2000)
[2]Zhao, Wei, Yang, and Chou, Phys. Rev. Lett. 92, 236805 (2004)
[3]Wimmer, Krakauer, Weinert, and Freeman, PRB 24, 864 (1981)

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