Quantum Size Effect in the Electronic Properties of Silicon Nanowires

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By using first-principles pseudopotential methods, we have studied the electronic properties of hydrogen-passivated silicon nanowires along [100], [110] and [111] directions with diameter up to 3.4 nm. It is found that as the diameter decreases, the energy band gaps are distinctly enlarged due to the quantum size effect. The valence band maximum moves down while the conduction band minimum moves up compared with the bulk. By using the many-body perturbation theory within the GW approximation, we have also investigated the self-energy correction to the energies of band edge states. Our calculation results show that he GW corrections are strongly size and orientation dependent. The effective masses as a function of diameter are also discussed.