عنوان مقاله:

The Role of Hydrogen on Dielectric Properties of Silicon Nanoclusters

محل انتشار:

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خلاصه مقاله:

computer simulation using pseudo-potential approach is carried out to investigate the band gap as a function of the size and the shape of small silicon quantum dots (called Si nanoclusters) having 3 to 44 atoms per dot with and without surface passivation by hydrogen. An empirical pseudo-potential Hamiltonian, a plane-wave basis expansion and a basic tetrahedral structure with undistorted local bonding configurations are used. In our simulation, the structures of the quantum dots are relaxed and optimized before and after hydrogen passivation. It is found that the gap increases more for hydrogenated surface than unpassivated one. Thus, both quantum confinement and surface passivation determine the optical and the electronic properties of Si quantum dots. Visible luminescence is probably due to radiative recombination of electrons and holes in the quantum-confined nanostructures. The effect of passivation of the surface dangling bonds by hydrogen atoms and the role of surface states on the gap energy is also examined. We investigate the entire energy spectrum starting from the very low-lying ground state to the very high-lying excited states. The results for the sizes of the gap, the DOS and the dielectric function of the size are presented. The importance of the confinement and the role of hydrogen passivation on the optical effects are discussed

کلمات کلیدی:

Pseudopotential, Quantum dots, Confinement, Passivation, Luminescence