ABSTRACT:

Electronic and optical properties of small silicon quantum dots having 3 to 44 atoms per dot with and without surface passivation are investigated by computer simulation using the pseudo-potential approach. An empirical pseudo-potential Hamiltonian, a plane-wave basis expansion and a basic tetrahedral structure with undistorted local bonding configurations are used. The structures of the quantum dots are relaxed and optimized before and after hydrogen passivation. It is found that the gap increases more for a hydrogenated surface than the unpassivated one. Thus, both quantum confinement and surface passivation determine the optical and electronic properties of Si quantum dots. Visible luminescence is probably due to the 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. The results for the density of states, the dielectric function, the frequency dependent optical absorption cross section, the extinction coefficient and the static dielectric constants of the size are presented. The importance of the confinement and the role of surface passivation on the optical effects are discussed.