

Light Emission Due to the Quantum Confinement of Carriers in Silicon-Based Nanostructures

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In the field of Si nanoscale ultralarge-scale integration, the quantum confinement effects is undesirable with respect to the characteristics and performance because the carriers are entirely confined in nanoscale or low-dimensional structures. Significant efforts are being made with regard to the positive use of the quantum confinement effect in Si nanoscale structures. One such attempt is related to the use of Si optoelectronics and photonics for optical interconnections within a Si chip. In this study, the intrinsic electronic structures in the Si-based nanostructures with different dimensions and sizes as candidates for Si optoelectronics were investigated by the DV- $X\alpha$ molecular orbital calculation, which is advantageous to simulate the valence band structures for nanomaterials. We discuss the shift of a light emission peak to a higher energy due to the quantum confinement of carriers in the Si-based nanostructures, which depends on the sizes and numbers of structural dimensions, on the basis of the calculated results. Also, effect of doping of group IIIB and VB elements in the periodic table on the extrinsic electronic structures of the Si-based nanostructures were clarified by combining the Vienna ab-initio code for determining the relaxation structures around the dopants with the DV- $X\alpha$ method for simulating the valence band structures. The results obtained are useful as a measure of possibility of the Si-based nano-structured materials for optoelectronics.