Quantum-Confinement Effects on Oscillator Strength in ZnO Quantum Dots

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Abstract

We present a theoretical investigation of the quantum confinement effects (QC) on the electronic and optical properties of ZnO quantum dots (QDs) embedded in MgO matrix. The latter material acts a huge barrier for both electrons and holes so that the ZnO QD behaves as a three-dimensional quantum well. MgO plays a role in the complete passivation of dangling bonds in a similar way of passivated nano-clusters. As a computational method, the tight-binding with sp^3s^*, with inclusion of spin-orbit interaction, is employed to probe the electronic band structure and inspect the number and the confinement energies of the bound states versus QD size (up to 20 Å) and the valence band offset (VBO). Excellent agreement is achieved between the theoretically obtained band-gap energy (Eg) and the available experimental photoluminescence (PL) data, especially when VBO = 1 eV, which correspond to the maximum compromised confinements between holes and electrons. Furthermore, theoretical results show that the QC energy follows a power-law rule, indicating strong confinement, and is the main reason behind the UV emissions in ZnO QDs. The strong QC character and the high binding energy of excitons would further explain the enhancement of the oscillator strength and recombination rate. The excellent agreement between our results and the available experimental data do corroborate our claims.