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Quantum-Confinement Effects on Optoelectronic Properties of ZnO Quantum Dots NACIR TIT, Physics Department, UAE University — We present a theoretical investigation on the optoelectronic properties of ZnO quantum dot (QD) embedded in MgO matrix. This latter material acts as huge barrier for both electrons and holes so that the ZnO QD behaves as a three-dimensional quantum well. As a computational method, the tight-binding with sp^3 minimal basis set is employed to probe the electronic band structure and inspect the number and confinement energies of the bound states versus QD size (up to 20 Å) and the valence band offset (VBO). Excellent agreement is achieved between theoretically obtained band-gap energy (E_g) and 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 quantum confinement (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 of excitons would further explain the enhancement of the oscillator strength and recombination rate. The excellent obtained agreements between our results and the available experimental data do corroborate our claims.

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