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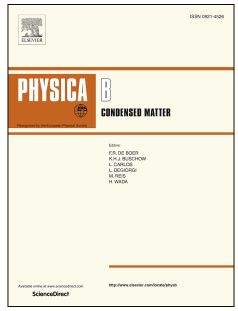

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Quantum Confinement Induced Shift in Energy Band Edges and Band Gap of a Spherical Quantum Dot

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Abstract

We have proposed and validated an ansatz as effective potential for confining electron/hole within a spherical quantum dot in order to understand quantum confinement and its consequences associated with energy states and band gap of Spherical Quantum Dots. Within effective mass approximation formalism, we have considered an ansatz incorporating a conjoined harmonic oscillator and Coulomb interaction as the effective potential for confining an electron or a hole within a spherical quantum dot and by employing appropriate boundary conditions, we have calculated the shifts in energy of minimum of conduction band (CBM) and maximum of valence band (VBM) with respect to size of spherical quantum dots. We have also determined the quantum confinement induced shift in band gap energy of spherical quantum dots. In order to verify our theoretical predictions as well as to validate our ansatz, we have performed phenomenological analysis in comparison with available experimental results for quantum dots made of CdSe and observe a very good agreement in this regard. Our experimentally consistent theoretical results also help in mapping the probability density of electron and hole inside a spherical quantum dot. The consistency of our results with available experimental data signifies the capability as well as applicability of the ansatz for the effective confining potential to have reasonable information in the study of real nano-structured spherical systems.

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