Shape and Size Effects on Energy Levels of Semiconductor Quantum Dots

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Semiconductor quantum dots or nanoparticles have found use in several nanotechnology applications, such as sensors, microlasers, and light-emitting diodes. Near-spherical quantum dots can be prepared using chemical and physical means. In this work the energy levels are calculated for HgTe, CdTe, and CdSe nanoparticles of various sizes using spherical infinite well and finite well models, with the height of the well being 5 eV for the HgTe finite well case. During preparation, slight deformations in the spherical shape of these quantum dots can occur. These are treated as perturbations to the spherical well models. For various values of deformation or ellipticity the energy level shifts for prolate and oblate quantum dots, with respect to spherical quantum dots, are calculated and compared with the literature available. The optical absorption and emission energies are also calculated for various sizes and spheroidal shape deformations of the quantum dots. Significant shifts in energy levels and transition energies due to shape deformation are found. Deformation leads to the lifting of degeneracy in the energy levels, to additional transitions in the absorption and emission spectra, and perhaps to the formation of long lived electron-hole pairs. Other effects, like Coulombic and exchange interactions, and surface states, could be taken into account as further perturbations to this model, which applies to quantum dots in the strong-confinement limit.