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A charge patching method calculation of a quantum dot/quantum well nanosystem.

First principles density functional calculations typically involve finding self-consistent solution to the Kohn-Sham equations, scaling with the cube of system size. To study large systems, such as semiconductor nanocrystals, an approximate ab initio potential may be constructed by patching together local charge motifs determined from self-consistent calculations on small prototype systems, and the eigenvalues determined using the folded spectrum method for a few band-edge states. In this talk, I will discuss the recent applications of this method to CdS/CdSe/CdS colloidal quantum dot quantum wells. Results on the effect of core, well, and shell thicknesses on the wavefunction and optical properties will be discussed. We find the conduction band wavefunction to be significantly less confined to the CdSe quantum well layer than predicted by k.p theory, and discuss the implications of this result on the theoretical interpretation of recent time-resolved Faraday rotation experiments. We will also briefly discuss the extensions of this approach to the explicit treatment of surface ligand effects and transition-metal doped nanocrystals.

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07.7.6 Computational Nanoscience
Semiconductors: 02.4 Electronic Structure & Optical Properties