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Investigation of Exciton States in CdSe Quantum Dots via Hamiltonian Diagonalization Method ZACHARY SCHULTZ, JOHN ESSICK, Reed College, Physics Department, Portland, OR 97202 — We analyze the electron-hole ("exciton") states involved in visible-light absorption by a spherical CdSe quantum dot. Working within the effective mass approximation and assuming a dot size on the order of the bulk exciton Bohr radius a_B , we exploit a Hamiltonian diagonalization method, which accounts for the exciton's kinetic T, direct Coulomb U_{eh} , and surface polarization U_p energies. Using a basis set composed of 54 composite infinite spherical-well wavefunctions, we obtain representations of exciton wavefunctions and their corresponding energies. For a dot radius $R = 0.80a_B$, we find that the energies associated with T, U_{eh} , and U_p are $+15.4E_R$, $-4.7E_R$, and $+1.4E_R$, where E_R is the bulk CdSe exciton Rydberg energy. Our theoretical results are then used to predict the size-dependent visible-light absorption spectra of CdSe quantum dots. Comparisons of the theoretical spectra are made to absorption data we have taken on CdSe dots with known radii. We find that our theoretical model accurately describes the experimental data for dots with radii $R \ge 0.6a_B$. Finally, we explain why our model breaks down for dots with $R \leq 0.6a_B$ and comment on the accuracy obtained with use of a more limited basis set.

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