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Size-dependent optical spectrum of CdSe nanocrystals W. JASKOLSKI, Instytut Fizyki UMK, Torun, Poland, G.W. BRYANT, J.G. DIAZ, NIST, Gaithersburg, MD 20899-8423 — An empirical sp^3d^5 tight-binding model has been employed to describe the optical properties of CdSe nanocrystals over a wide range of sizes. The sp^3d^5 model explains successfully the single-particle electron levels and excitonic effects including the evolution of both the emission and absorption peaks with confinement. We provide an interpretation of the band-edge fine structure in agreement with both the one- and two- photon spectroscopies and the PLE resonant and non-resonant Stokes shifts. Previous effective mass, pseudopotential and sp^3s^* tight-binding models were unable to explain such experiments. The wurtzite lattice structure splits the lowest S- and P- hole states into two doublets that overlap, in accordance to the indistinguishability observed between the one-photon and two-photon spectroscopies. A correct description of the spin-orbit coupling allows the non-resonant Stokes shift to be reproduced. Finally, for dot radius below 2.3 nm, an optically passive $P-$ level becomes the ground hole state giving rise to the large resonant Stokes shift observed experimentally.

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