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Atomistic calculations of the biexciton fine structure in CdSe nanocrystals O. VOZNYY, M. KORKUSINSKI, E. KADANTSEV, P. HAWRYLAK, Institute for Microstructural Sciences, National Research Council, Ottawa, Canada — We present an atomistic tight-binding (TB) theory of exciton (X) and bi-exciton (XX) confined in CdSe spherical nanocrystals, of fundamental interest for multi-exciton generation applications. The single-particle electron (e) and hole (h) states are computed using an atomistic 20-band TB model accounting for the crystal field splitting and with a model surface passivation. The optically excited states are expanded in e-h configurations and the many-body spectrum is computed in the configuration-interaction (CI) approach accounting for the Coulomb mixing between X and XX configurations. The emission and absorption spectra are obtained using the Fermi's Golden Rule. We find that the electronic and optical properties of X and XX are determined by the hole spectrum being composed of four quasi-degenerate low-lying states well separated from the rest of spectrum. As a consequence, the X and XX present manifolds of states, whose structure is determined by electron-hole exchange for X, and by correlation effects for XX. This results in a fine structure of XX optical spectra. We also treat the mixing between X and XX in an exact manner in CI approach. We find that in CdSe nanocrystals it is weak, resulting only in minor shifts of intensity and a small line broadening of emission spectra.

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