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Radiative recombination of charged excitons and multiexcitons in CdSe quantum dots M. CLAUDIA TROPAREVSKY, ALBERTO FRANCESCHETTI, Oak Ridge National Laboratory, Oak Ridge TN 37831 — Radiative recombination of neutral and charged biexcitons has been recently observed in CdSe nanocrystals using time-resolved, femtosecond spectroscopy. Here we report semi-empirical pseudopotential calculations of charged exciton and multiexciton emission spectra of CdSe nanocrystals. We studied the mono-exciton X (one electron, one hole, 1e-1h), the charged excitons X^- (2e-1h) and X^+ (1e-2h), and the charged biexcitons XX^- (3e-2h) and XX^+ (2e-3h). For a 3.9 nm-diameter CdSe nanocrystal, we found that the emission peak for the X^- recombination overlaps with that of X (at 2.16 eV), while the X^+ emission peak is slightly blue-shifted (by 0.02 eV). We also found that the main peaks in the XX^- and XX^+ emission spectra are significantly blue-shifted with respect to the exciton peak X (by 0.04 and 0.05 eV, respectively) because of inter-particle interactions. In the case of XX^- , we observe an additional peak of lower intensity at 2.50 eV originating from the recombination of a 1p electron state with a partially occupied 1p hole state. This work was supported by the US DOE Office of Science LAB3-17 initiative.

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