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Size and shape dependence of CdSe nanocrystal band-edge exciton fine structure* QINGZHONG ZHAO, KWISEON KIM, PETER A. GRAF, WESLEY B. JONES, ALBERTO FRANCESCHETTI, National Renewable Energy Laboratory, LIN-WANG WANG, Lawrence Berkeley National Laboratory — Advances in growth methods of nanocrystals led to controlled synthesis over size and shape, influencing their optical properties. Ground exciton states of CdSe nanocrystals are shown to be sensitive to their geometries. We investigate the exciton fine structure of CdSe nanocrystals using empirical pseudopotential and configuration interaction methods[1,2]. Systematic studies of the size and shape dependency are performed on the band edge states of CdSe spherical quantum dots, elongated nanorods, flattened nanodisks, nanowires and quantum wells. Large-scale electronic calculations consisting of 100–20,000 atoms with diameters from 2 to 8 nm and lengths from 2 to 11 nm were carried out. We explore size and shape dependence of exciton fine structure over the diameter-length space and explain it by the interplay of quantum confinement, crystal field splitting, and exchange interaction. We find the experimentally observed dark-bright exciton crossing[3] and discuss its size-shape dependency. [1] L. W. Wang and A. Zunger, *Phys. Rev. B* **51**, 17398 (1995). [2] A. Franceschetti, *et al.*, *Phys. Rev. B* **60**, 1819 (1999). [3] N. Le Thomas, *et al.*, *Phys. Rev. Lett.* **94**, 016803 (2005). *This work was supported by US DOE-SC-BES and ASCR TMSN Initiative.

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