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Theoretical investigation of the high energy excitations in silicon nanocrystals ADAM GALI, MARTON VOROS, Budapest University of Technology and Economics, DARIO ROCCA, GERELY ZIMANYI, GIULIA GALLI, UC Davis — Recently, efficient multi-exciton generation (MEG) has been reported for several nanoclusters including silicon nanocrystals (SiNC), too. However, the existence of MEG has been disputed in the literature. The reported bi-exciton states in SiNC involve high energy empty states of SiNC. These states are expected to be very delocalized, and thus easily modified by the environment surrounding the SiNCs. In addition, the SiNCs are fabricated in a solution that usually contains CnHm molecules, e.g. hexane, that may bind to the surface of SiNCs, and modify their absorption spectrum. We have studied the absorption spectra of hydrogenated SiNCs by first principles calculations. The geometry was optimized within density functional theory (DFT), while absorption spectra were determined by time-dependent DFT. The effect of the environment on the SiNC was modeled by i) varying the distance between the nanoparticles ii) allowing for surface reconstruction and iii) monitoring the effect of absorption of CnHm groups on absorption spectra. We found that the high energy spectrum of SiNCs strongly depends on the environment. Our findings indicate that taking into account effects of surface states and SiNCs concentration in solution is crucial, in order to understanding multi exciton generation.

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