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Density Functional Theory Investigation of Tunable Surface Composition of CdS Quantum Dots[1] OLEG PREZHDO, AMANDA NEUKIRCH, JEREMY YOUNG, HELEN WEI, CHRISTOPHER EVENS, TODD KRAUSS, University of Rochester — It has recently been observed that surface composition of CdS QDs greatly affects photoluminescence. Band edge emission is quenched in sulfur terminated CdS QDs and recovered when QDs were cadmium terminated. However, in all cases the absorption spectra remained relatively unchanged. To understand the origin of this phenomenon, the density of states in a stoichiometric, Cd rich, and S rich dots was investigated using density functional theory (DFT). It was found the in the S rich system states within the band gap were introduced, providing a channel for non-radiative electronic relaxation. Gap states were also introduced in the Cd rich system compared to the stoichiometric system, but a significant band gap remained in even the most Cd rich systems. Finally, time dependent (TD)DFT was used to calculate the spectra of the various systems. It was found that created gap states were largely optically inactive. Therefore the new states would not participate in optical absorption or emission, but could participate in electron phonon relaxation. This study clarifies the role of surface defects in QD optical properties and provides a route for tuning those optical properties by controlling surface composition.

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