Impact of the Thiol/Thiolate Passivation of CdS Quantum Dots on Their Optical Spectra

Alyssa Roberts,[1] Levi Lystrom,[1] Svetlana Kilina[1]

[1] Chemistry and Biochemistry Department North Dakota State University, Fargo, ND 58102

Using computations based on Density Functional theory (DFT) and time dependent DFT (TD-DFT), we investigate the effect of the interaction between the CdS quantum dot (QD) and passivating thiol ligands and their impacts on the optical spectra. We specifically focus on the effect of the conversion of thiol to thiolate with the proton moving either to the solution or to the surface sulfur of the QD. The nonpolar solvent propylamine whose effects on the thiol deprotonation process are compared to the polar solvent acetonitrile. Propylamine has a higher tendency to abstract the proton from thiol resulting in higher portion of thiolates and surface protons compared to those in acetonitrile. However, full thiol deprotonation decreases the optical intensity of lowest energy transitions of the QD. Our calculations provide insights into delicate interplay within a light emitting diode. The information gathered from this research could be used towards furthering our understanding of optical properties of QDs.