# Nanoscale Photovoltaics: Aminoethanethiol Coated CdSe Quantum Dots

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Ordered heterojunction solar cells show promise for the development of next generation high efficiency photovoltaics due to their optimized carrier transport properties. One approach is to use colloidal CdSe quantum dots (QD) to decorate long and aligned carbon nanotubes. In principle, this choice combines the tunable band gap and multiple exciton generation of the QDs with the high carrier mobility of carbon nanotubes. One difficulty involves the proper surface capping of the QD and its attachment to the nanotube. QD capping agents typical consist of long carbon chains which form a barrier to charge carriers and hinder charger transfer. Short ligands such as aminoethanethiols and pyridines are thus a present focus of activity. Using first principles, we provide insights into binding of the aminoethanethiol molecules to the QD surface. The linking end of the aminoethanethiols contains a sulfur atom with an unpaired electron: the sulfur acts either as a hole donor to the QD when a Cd-S bond forms or as an electron donor when a S-Se bond forms. While the S-Cd bond is stronger in isolation, the preferred binding morphology for two ligands involves both S-Cd and S-Se bonds. We discuss these and related issues and their implications.

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