

Abstract Submitted
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**Interaction of Phenylthiocarbamates and Hydrides With CdSe
Quantum Dots and its Effect on their Optical Response¹** SVETLANA

KILINA, North Dakota State University — Using DFT and TDDFT, we study the effect of surface anionic ligands, such as hydrides and phenylthiocarbamates (PTC), on the photophysics of quantum dots (QDs). Hydrides strongly enhance the emission of CdSe QDs, although the mechanism of such enhancement is unclear. Our simulations show that H⁻ removes surface Se ions responsible for trap states, which explains increased emission after hydride treatment. PTC are commonly used ligands for passivating QDs that enhance their conductivity and redshift optical spectra, while no reports have been focused on the ligand exchange chemistry itself. Our calculations demonstrate that PTC ligand exchange with CdSe QDs is a more complex process than was initially thought, in which ligand decomposition competes with ligand exchange. In addition, we found that solvent polarity governs PTC deprotonation. In nonpolar solvents, some part PTC loses their protons, which are bound to the Se sites. However, and no such deprotonation is observed in polar solvents. Fully protonated PTC bound to the QD surface lead to appearance of trap states with low optical activities. In contrast, partial deprotonation of PTC results in the lowest energy optically active transitions leading to improved emission of QDs.

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