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Ligand Interface Chemistry of Lead Chalcogenide Nanocrystals[1]

KUN LIU, Cornell, CLIVE BEALING[2], University of Connecticut, RICHARD HENNIG, Cornell, HENNIG GROUP TEAM — Lead chalcogenides nanocrystals (NCs) have shown promise in photovoltaic applications. Surface chemistry is one of the most important, yet least understood aspects of NC synthesis and functionalization controlling their properties. For example, an incomplete surface passivation could create trap states that enhance undesired exciton recombination. Clever choices of ligands ensure that neighboring NCs are electronically coupled while maintaining their quantum size effects. These two barriers limiting performance of NC solar cells illustrate the importance of fundamental studies for the interaction between ligands and NC surfaces. We use density functional theory to determine the binding sites and energies of ligands commonly used in NC synthesis and functionalization. Specifically we study amine-, carboxyl-, and thiol-ligands on different PbSe and PbS surfaces. For methylamine ligands we find a similar binding energy on the (100) and (111) facet while carboxylic acid ligands strongly prefer the (111) facet leading to different effective NC shapes.

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[2] This work was done when Clive was at Cornell

Kun Liu
Cornell

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