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Surface states in CdSe nanocrystals with carboxylic acid ligands: an ab initio study[1] OLEKSANDR VOZNYY, Quantum Theory Group, Institute for Microstructural Sciences, NRC Ottawa, Canada K1A 0R6 — The electronic properties of the realistic Cd-rich CdSe quantum dots with covalently bound (X-type) carboxylic ligands are investigated using density functional theory for the nanocrystal (NC) sizes sufficient to distinguish core and surface states. We find that Cd and Se atoms with only one dangling bond do not create surface traps. The amount of ligands and the crystal shape is dictated by the overall electronic balance of the NC rather than by the surface free energies of particular ligated facets. To achieve this balance more ligands are required than there are "ideal" adsorption sites for them, creating ligand-induced trap states near the valence band maximum. These extra ligands are mobile on surface, resulting in spectral diffusion of the trap levels, providing first atomistic example of diffusion and activated recombination centers models for blinking.

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