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Ab-Initio Calculations of the Structural Properties of CdSe Nanorods and their Interaction with Organic Ligands ANDREW WILLIAMSON, AARON PUZDER, GIULIA GALLI, Lawrence Livermore National Laboratory, LIBERATO MANNA, PAUL ALIVISATOS, Lawrence Berkeley Laboratory — First principles electronic structure simulations are used to study the atomistic detail of the interaction between organic surfactant molecules and the surfaces of CdSe semiconductor nanoparticles.[1] These calculations provide insights into the relaxed atomic geometry of organics bound to semiconductor surfaces at the nanoscale as well as the electronic charge transfer between surface atoms and the organics. We calculate the binding energy of phosphine oxide, phosphonic and carboxylic acids and amine ligands to a range of CdSe nanoparticle facets. The calculated relative binding strengths of ligands to different facets support the hypothesis that these binding energies control the relative growth rates of different facets, and therefore the resulting geometry of the nanorods. The calculated relaxed atomic geometries of CdSe nanorods with a range of diameters and growth directions are then compared with the results of EXAFS measurements of recently synthesized nanorods to determine their atomic structure and surface relaxations. [1] A. Puzder, A.J. Williamson, N. Zaitseva, G. Galli, L. Manna and A.P. Alivisatos, Nano Lett. (2004).

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