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Analysis of the effects of surface chemistry on the XAS spectra of CdSe nanomaterials HEATHER WHITLEY, Lawrence Livermore National Laboratory, DAVID PRENDERGAST, Lawrence Berkeley National Laboratory, TADASHI OGITSU, ERIC SCHWEGLER, Lawrence Livermore National Laboratory — X-ray absorption spectroscopy (XAS) is an element-specific probe of local electronic structure, and is an ideal method to analyze chemical bonding. We investigate the consistency of theoretically predicted structures of CdSe nanomaterials with recently measured XAS via *ab initio* calculations. Using plane-wave DFT, the x-ray absorption cross-section for the Cd L_3-edge of small CdSe clusters with a variety of surface ligands is calculated. We also highlight the importance of including excitonic effects in our simulations of core excitation spectra. We compare our simulations to existing experimental data on the ligand dependence of XAS for ligated quantum dots up to $\sim$3nm in diameter. Based on the favorable comparison of our theoretical spectra with experimental measurements, we infer the validity of our DFT-derived structure and surface passivation for these quantum dots and its relevance to understanding optoelectronic properties of solution-synthesized CdSe nanocrystals. Prepared by LLNL under Contract DE-AC52-07NA27344.

Heather Whitley
Lawrence Livermore National Laboratory

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