Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

***Ab Initio* Study of the Effects of Surface Chemistry and Size on Xray Absorption Spectra of CdSe Nanoparticles** HEATHER WHITLEY, Lawrence Livermore National Laboratory, Livermore, CA 94551, DAVID PRENDERGAST, Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, TADASHI OGITSU, ERIC SCHWEGLER, Lawrence Livermore National Laboratory, Livermore, CA 94551 — The specificity of their opto-electronic properties with respect to size, shape, and surface chemistry, as well as cost-effective solution based methods of synthesis, make CdSe nanoparticles a material of choice for use in novel opto-electronic devices, such as photovoltaics and field effect transistors. Developing methods by which these nanomaterials can be systematically engineered to meet specific device goals is largely dependent on understanding how surface passivation and reconstruction affect the properties of a given nanomaterial. Xray absorption spectroscopy (XAS) is an ideal method for structural analysis, but its application to studying nanomaterial surfaces is nontrivial due to the convolution of the absorption of surface atoms with those within the nanomaterial. We utilize *ab initio* methods to investigate the dependence of the Cd L-edge xray absorption cross-section on the size and passivation for Cd atoms both at the surface and within the core of CdSe nanomaterials. We aim to enable routine surface characterization of CdSe nanomaterials via XAS. Prepared by LLNL under Contract DE-AC52 07NA27344.

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Date submitted: 20 Nov 2008 Electronic form version 1.4