

Abstract Submitted  
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**First-principles spectroscopic characterization of PbSe nanoparticles passivated with Fe complexes** KEITH GILMORE, AARON HAMMACK, APRIL SAWVEL, EVELYN ROSEN, D. FRANK OGLETREE, JEFFREY URBAN, DELIA MILLIRON, BRETT HELMS, BRUCE COHEN, DAVID PRENDERGAST, Lawrence Berkeley National Lab, THE MOLECULAR FOUNDRY TEAM — Given that defining characteristics of nanoparticles – morphology, catalytic reactivity, optical and electronic properties – are often dictated by their surfaces, it is informative to investigate how surface chemistry and structure change as different ligands are introduced to the surface. Starting with oleate-passivated PbSe nanoparticles, we remove the oleate ligands and replace them with an organometallic complex: cyclopentadienyl iron dicarbonyl. Measured and calculated x-ray photoemission core-level shifts indicate a charge transfer between surface Pb atoms and Fe atoms. We investigate the nature of this charge transfer in more detail through analysis of x-ray absorption spectra (XAS) at the Fe L-edge. Fe XAS are calculated from first-principles using a GW-based Bethe-Salpeter approach. The spectra reveal that the extent to which pi-backbonding is possible between the Fe and associated carbonyls varies with the charge density on the Fe atom.

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