

Abstract Submitted  
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**Theory of Energy Level Tuning in Quantum Dots by Surfactants** DANYLO ZHEREBETSKYY, LIN-WANG WANG, Materials Sciences Division, Lawrence Berkeley National Laboratory, MATERIALS SCIENCES DIVISION, LAWRENCE BERKELEY NATIONAL LABORATORY TEAM — Besides quantum confinement that provides control of the quantum dot (QD) band gap, surface ligands allow control of the absolute energy levels. We theoretically investigate energy level tuning in PbS QD by surfactant exchange. We perform direct calculations of real-size QD with various surfactants within the frame of the density functional theory and explicitly analyze the influence of the surfactants on the electronic properties of the QD. This work provides a hint for predictable control of the absolute energy levels and their fine tuning within 3 eV range by modification of big and small surfactants that simultaneously passivate the QD surface.

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