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Energy level modification in lead sulfide quantum dot photovoltaics through ligand exchange PATRICK BROWN, DONGHUN KIM, Massachusetts Institute of Technology, RICHARD LUNT, Michigan State University, MOUNGI BAWENDI, JEFFREY GROSSMAN, VLADIMIR BULOVIC, Massachusetts Institute of Technology — The electronic properties of lead sulfide colloidal quantum dots (PbS QDs) can be controlled through modification of QD size and surface chemistry. Novel surface passivation techniques involving organic or inorganic ligands have contributed to a rapid rise in the efficiency of QD photovoltaics, yet the influence of ligand-induced surface dipoles on PbS QD energy levels and photovoltaic device operation is not yet completely understood. Here, the valence band energies of PbS QDs treated with twelve different ligands are measured using ultraviolet photoelectron spectroscopy (UPS), and a valence band shift of up to 0.75 eV is observed between different ligand treatments. Atomistic simulations of ligand binding to pristine PbS(100) and PbS(111) slabs qualitatively reproduce the measured energy level shifts. 1,2-benzenedithiol and 1,3-benzenedithiol treatments, which result in valence band energies differing by ~ 0.2 eV, are employed for PbS QDs in three different solar cell architectures, and changes in device performance are correlated with the measured energy level shift. These findings complement the known bandgap-tunability of colloidal QDs and highlight an additional level of control over the electronic properties of PbS QDs.

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