Supporting Information for:

Targeted Ligand Exchange Chemistry on Cesium Lead Halide Perovskite Quantum Dots for High-Efficiency Photovoltaics

Lance M. Wheeler,¹* Erin M. Sanehira,^{1,2} Ashley R. Marshall,^{1,4} Philip Schulz,^{1,5} Mokshin Suri,³ Nicholas C. Anderson,^{1†} Jeffrey A. Christians,¹ Dennis Nordlund⁶, Dimosthenis Sokaras⁶, Steven P. Harvey,¹ Joseph J. Berry,¹ Lih Y. Lin,² and Joseph M. Luther¹*

¹National Renewable Energy Laboratory, Golden, CO, 80401, USA

²Department of Electrical Engineering, University of Washington, Seattle, WA 98195, USA

³McKetta Department of Chemical Engineering and Texas Materials Institute, The University of Texas at Austin, Austin, Texas 78712-1062

⁴Department of Chemistry and Biochemistry, University of Colorado, Boulder, CO, 80309, USA

⁵CNRS, Institut Photovoltaïque d'Île de France (IPVF), UMR 9006, 91120 Palaiseau, France

⁶Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA

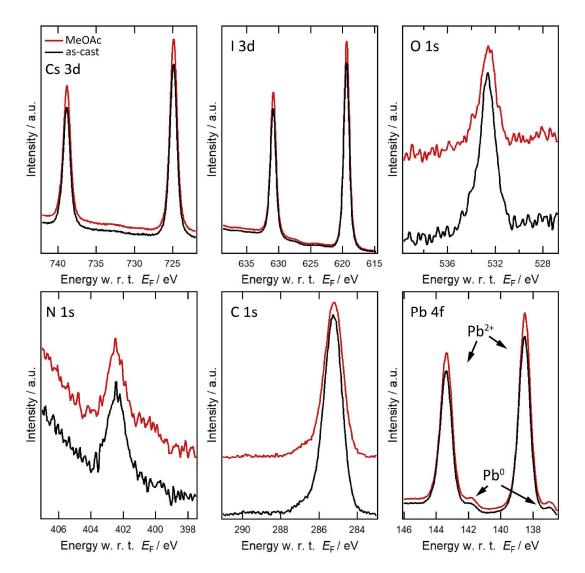


Figure S1. XPS core level spectra of CsPbI₃ QD thin-films before and after treatment with saturated $Pb(NO_3)_2$ in MeOAc. Prolonged exposure to X-rays during the XPS measurements lead to the emergence of a small metallic lead (Pb⁰) contribution.

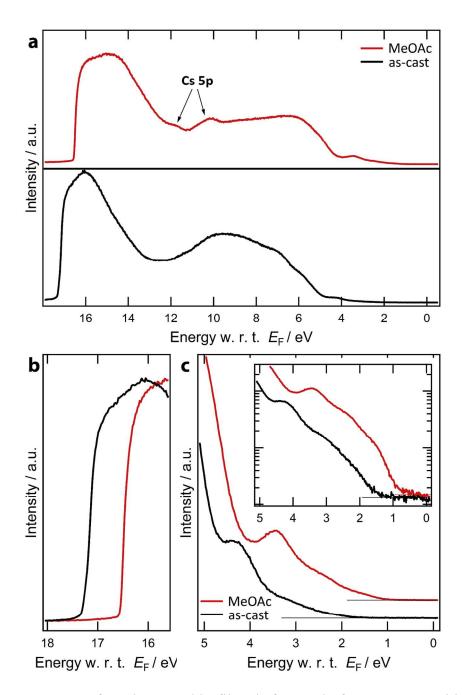


Figure S2. UPS spectra of $CsPbI_3$ QD thin-films before and after treatment with MeOAc. (a) Survey scan, (b) secondary electron cut-off, and (c) valence band region (inset in semilogarithmic scale). An apparent change of the work function by over 0.7 eV is accompanied by a concomitant shift in the valence band onset, which could be related to charging or pronounced surface band bending during the measurement as a function of surfactant coverage.

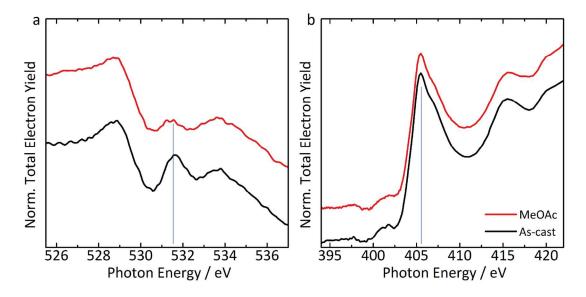


Figure S3. Soft X-ray XAS spectra of CsPbI₃ QD thin-films before and after treatment with MeOAc at the (a) oxygen K-edge and (b) nitrogen K-edge. Vertical lines act as guide to the eye and mark the principal spectra fingerprints of carboxylate (carboxyl) and ammonium moieties, respectively.

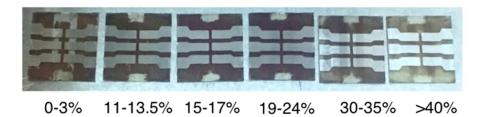


Figure S4. Labels below the image indicate the relative humidity (RH).

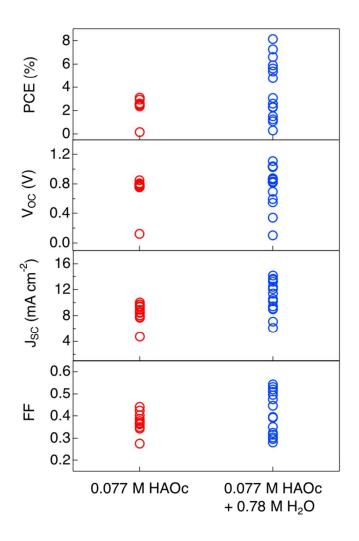


Figure S5. PV device statistics for samples fabricated with acetic acid and water incorporated into the film treatment solution.

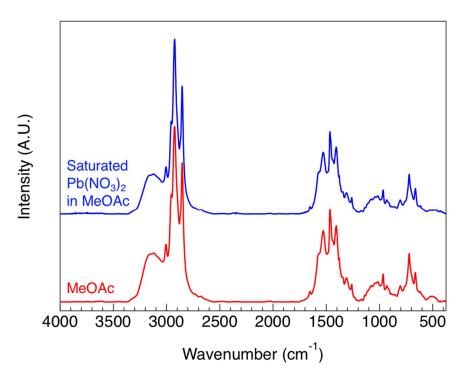


Figure S6. FTIR of CsPbI₃ QDs treated with neat MeOAc (red) and saturated $Pb(NO_3)_2$ in MeOAc

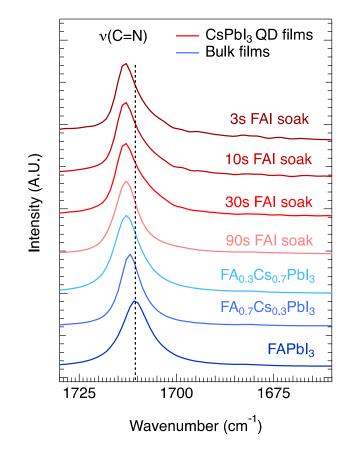


Figure S7. FTIR spectra highlighting the v(C=N) resonance that is blueshifted on the surface of QDs (shades of red) compared to the bulk films (shades of blue).

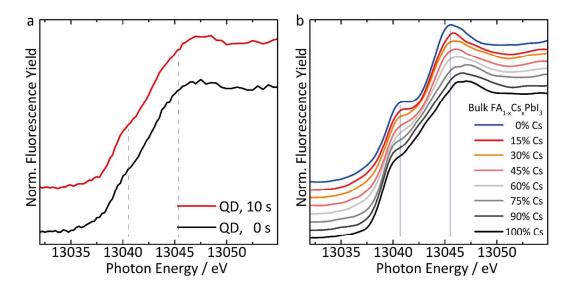


Figure S8. Hard X-ray XAS spectra of (a) CsPbI₃ QD thin-films after treatment with saturated $Pb(NO_3)_2$ in MeOAc and subsequent exposure to FAI in EtOAc (for 0 and 10 s, respectively), and of (b) bulk FA_{1-x}Cs_xPbI₃ thin-films for comparison. Vertical lines indicate distinct features corresponding to Pb coordinated in PbI₆ octahedra of FA rich thin-films.