Supporting Information

Thermal-Carrier-Escape Mitigation in a Quantum-Dot-In-Perovskite Intermediate Band Solar Cell via Bandgap Engineering

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5 pages. 2 equations and 7 figures.

Supporting Equations

The QD optical bandgap E_0 as a function of the QD diameter d in nm.

From: Moreels, I.; Lambert, K.; Smeets, D.; De Muynck, D.; Nollet, T.; Martins, J. C.; Vanhaecke, F.; Vantomme, A.; Delerue, C.; Allan, G.; Hens, Z. Size-Dependent Optical Properties of Colloidal PbS Quantum Dots. ACS Nano 2009, 3 (10), 3023–3030.

$$E_0 = 0.41 + \frac{1}{0.0252d^2 + 0.283d} \quad \text{(S1)}$$

The second state for electrons, or $1P_e$, in the MAPI-PbS QDs is obtained using Equation 1, reported for the $1S_e \rightarrow 1P_e$ transition in PbS QDs with iodide ligands, where d is the size (diameter) of the dots.

From: Ramiro, I.; Kundu, B.; Dalmases, M.; Özdemir, O.; Pedrosa, M.; Konstantatos, G. Size- and Temperature-Dependent Intraband Optical Properties of Heavily n-Doped PbS Colloidal Quantum Dot Solid-State Films. ACS Nano 2020, 14 (6), 7161–7169.

$$1P_e - 1S_e = \frac{1.57}{d} - \frac{2.5}{d^2} \quad \text{(S2)}$$

Supporting Figures

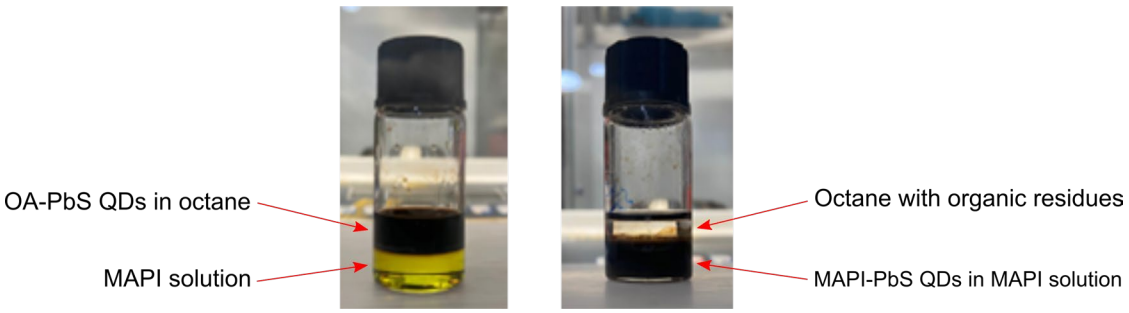

Figure S1. Pictures of CQD solutions before (left) and after (right) the ligand-exchange process.

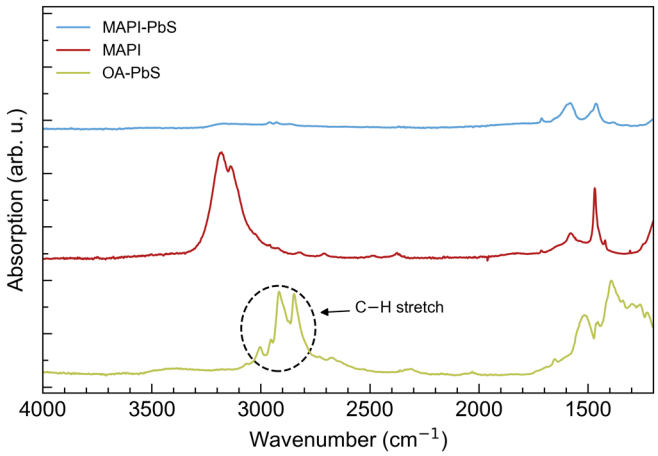

Figure S2. FTIR spectra of PbS QDs before (OA-PbS) and after (MAPI-PbS) the ligand exchange process, together with a reference MAPI film.

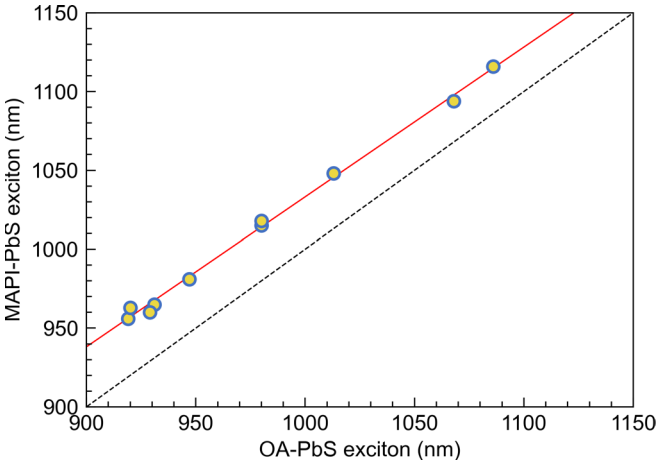

Figure S3. QD excitonic red-shit upon ligand exchange. The red line is a linear regression. The dashed black line marks the case without energy shift.

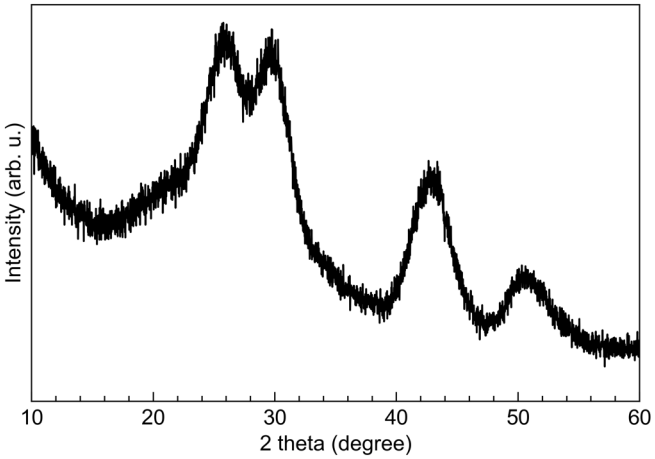

Figure S4. Typical XRD spectrum of OA-PbS QDs.

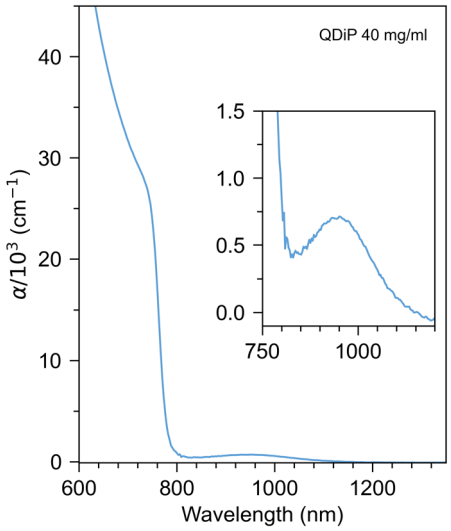

Figure S5. Absorption coefficient of a QDiP material with C_{QD} = 40 mg/ml.

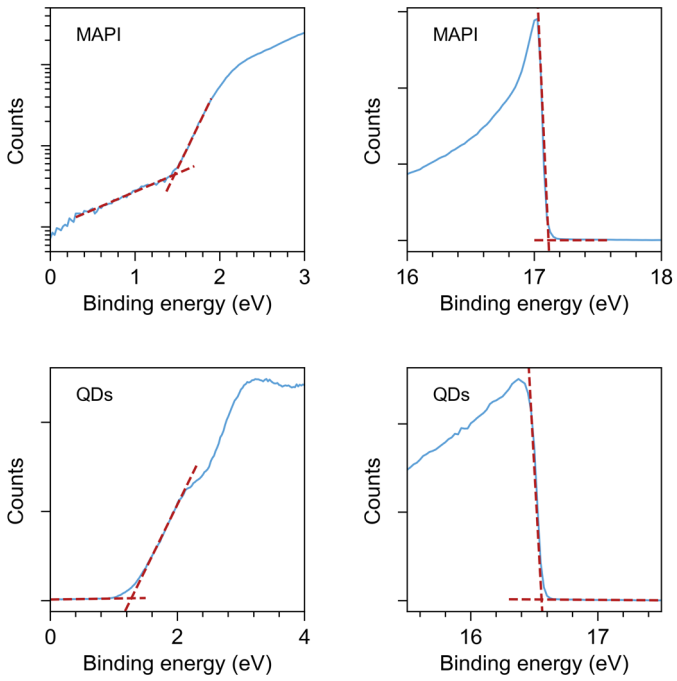

Figure S6. UPS data of a secondary electron cut-off (high-energy fit) and valence band (low-energy fit) of one of the MAPI and one of the MAPI-PbS QDs measured samples.

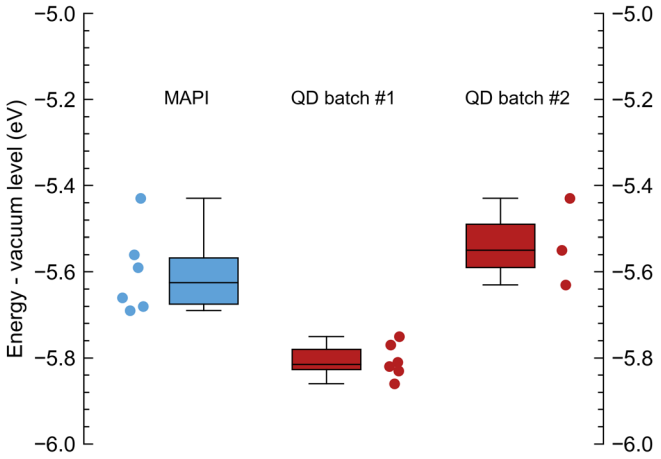

Figure S7. Energies obtained by fitting of the UPS results of the VB edge of MAPI and the $1S_h$ state of MAPI-PbS QDs like those used in the measured solar cell. The $1S_e$ energy used in Figure 4a of the main text is the average of the mean values of the two MAPI-QDs batches measured.