Sequential Solid-State Multiligand Exchange of FAPbI₃ Quantum Dots

for More Efficient and Stable Photovoltaic Devices

Mahdi Hasanzadeh Azar^{a, 1}, Habib Abdollahi^{b, 1}, Shaghayegh Arabloo^b, Abdolreza Simchi^{c,*}

^aDepartment of Engineering Physics, McMaster University, Hamilton, ON, Canada

^bAria Pyrex Laboratory Equipment and Materials Company, Tehran, Iran

^cFraunhofer Institute for Manufacturing Technology and Advanced Materials, 28359 Bremen,

Germany

¹ These two authors contributed equally.

Diffraction angle (2θ°)	Miller index
13.92	(100)
28.22	(200)
31.28	(012)
40.22	(220)
42.25	(221)

Table S1. Diffraction angles of alpha-phase of FAPbI₃ with their Miler plane index.



Figure S1. Tauc plot of UP FAPbI₃ CQDs.



Figure S2. Photographs taken from spin-coated films of (a) UP, (b) LP3H, and (c) LP3C QDs on FTO.

Wavenumber (cm ⁻¹)	Bonds	Belongs to
1717	v(C=N)	FA ⁺ in FAPbI ₃
3300 and 3500	-N-H	OAm and FAI
2919	CH ₂ Asymmetric	OA, OAm
2885	CH ₂ symmetric	OA, OAm
2984	CH ₃ symmetric	OA, OAm
1409	COO ⁻ symmetric	Oleate
1530	COO ⁻ Asymmetric	Oleate
2382 and 2412	S-H	MPA
3170	N-H ₃ ⁺	FA^+
3357	$C=N-H_2^+$	FAI

Table S2. All FTIR peaks and corresponding bonds of precursors.

Table S3. Integrated peak area (IPA) of ligands and FA⁺ deduced from ¹H NMR spectra

Sample	IPA of Ligands (×10 ⁹)	Ligand Removal	IPA of FA⁺ (×10⁷)
UP	2.27	0% (100% coverage)	1.67
LP3	1.089	52.02	1.09
SLP	0.352	84.49	0.67
SLP-MF	0.059	97.4	1.23

IPA: Integrated Peak Area

Table S4. The average characteristics of SLP and SLP-MF solar cells (n=10).

Cells	V _{OC} (V)	J _{SC} (mA/cm ²)	FF (%)	PCE (%)
R-SLP	1.038±0.03	10.91±0.8	65.75±2.3	7.48±1.0
R-SLP-MF	1.068 ± 0.01	13.49±0.5	71.94±1.18	10.38±0.7



Figure S3. The statistical distribution of photovoltaic parameters: (a) V_{OC} ; (b) J_{SC} ; (c) FF; (d) PCE



Figure S4. The effect of the SLP-MF QD film thickness on PCE.



Figure S5. The effect of MPA concentration on the PCE of cells at one mg FAI concentyration.



Figure S6. Absorbance spectrum of SLP and SLP-MF thin-films.



Figure S7. Representative top -view FESEM images of (a) SLP and (b) SLP-MF PQD layers.