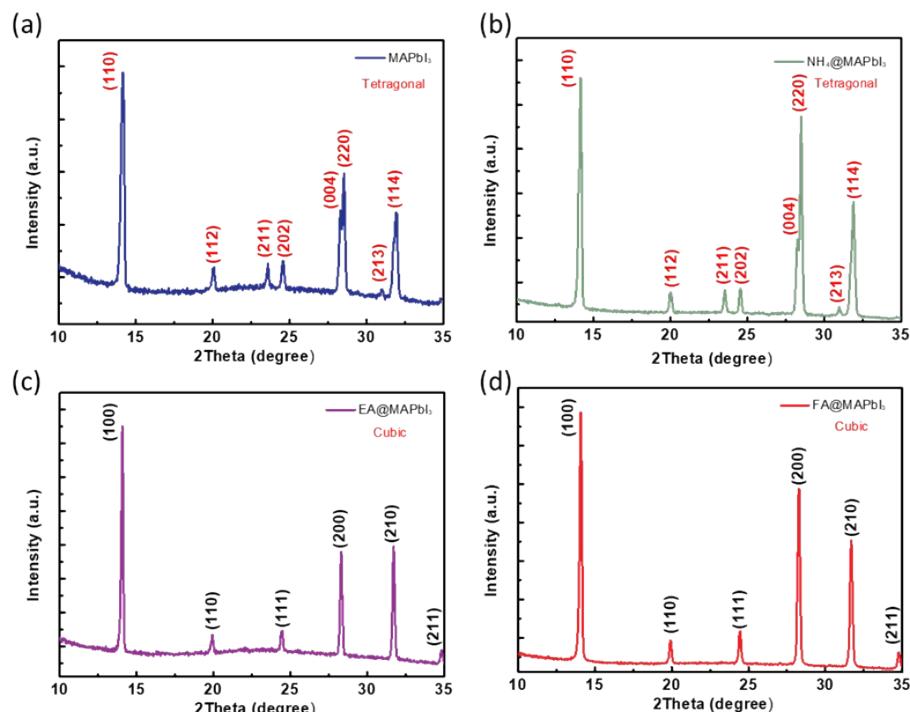


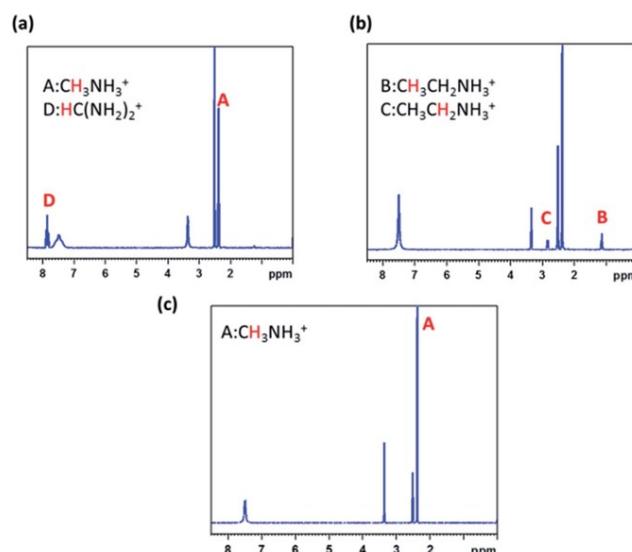
## Supporting Information for

### A Study on the Effects of Mixed Organic Cations on the Structure and Properties in Lead Halide Perovskite

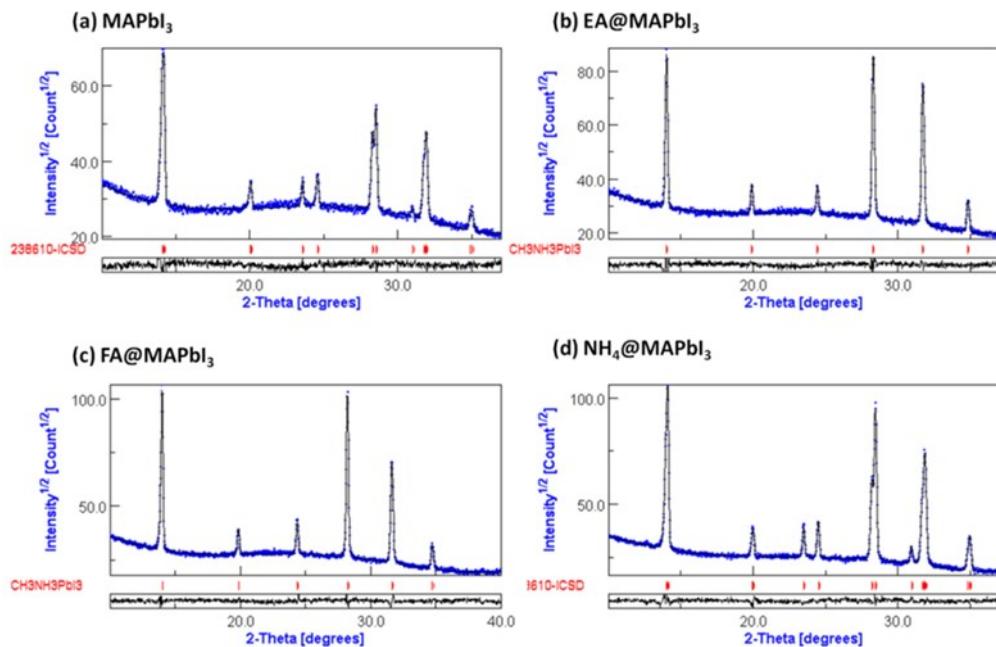
**Figure S1.** Powder XRD patterns of the perovskite crystals (a) MAPbI<sub>3</sub>; (b) NH<sub>4</sub>@MAPbI<sub>3</sub>; (c) EA@MAPbI<sub>3</sub>; (d) FA@MAPbI<sub>3</sub>



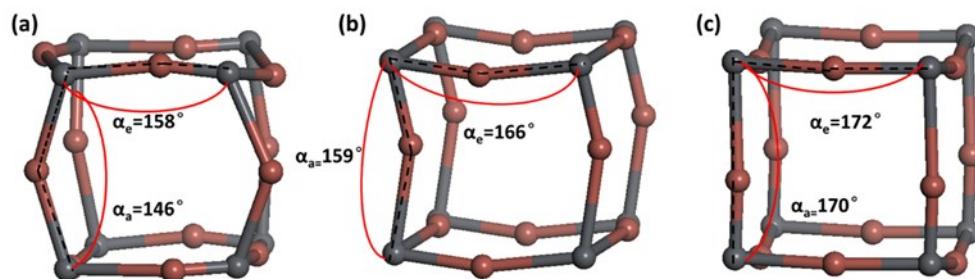
**SFigure 2.** <sup>1</sup>H NMR spectra of the samples, (a) EA@MAPbI<sub>3</sub>; (b) FA@MAPbI<sub>3</sub>; (c) MAPbI<sub>3</sub>.



**SFigure 3.** Rietveld refinements output plot using MAUD of samples (a) MAPbI<sub>3</sub>; (b) NH<sub>4</sub>@MAPbI<sub>3</sub>; (c) EA@MAPbI<sub>3</sub>; (d) FA@MAPbI<sub>3</sub>.



**SFigure 4.** Structure diagram of (a) NH<sub>4</sub>@MAPbI<sub>3</sub>; (b) MAPbI<sub>3</sub>; and (c) EA@MAPbI<sub>3</sub> crystals.



**Table1.** Fitting from Rietveld refinements with XRD data for the four samples determined by MAUD.

Parameter	MAPbI <sub>3</sub>	NH4@ MAPbI <sub>3</sub>	EA@ MAPbI <sub>3</sub>	FA@ MAPbI <sub>3</sub>
<b>Symmetry</b>	Tetragonal	Tetragonal	Cubic	Cubic
<b>Space group</b>	I4/mcm	I4/mcm	Pm-3m	Pm-3m
<b>a (Å)</b>	8.931	8.879	6.308	6.328
<b>b (Å)</b>	8.931	8.879	6.308	6.328
<b>c (Å)</b>	13.032	12.664	6.308	6.328
<b>sig</b>	1.19	1.57	1.64	1.44
<b>R<sub>w</sub> (%)</b>	4.04	4.56	5.43	4.91
<b>R<sub>p</sub> (%)</b>	3.39	2.28	3.91	3.43