Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Ion-exchange-induced $MAPbI_3$ thin-film 3D-2D and 3D-1D conversions: unveiling structural transformations in films via synergistic and competitive approaches

Shuhuang Chen,[a] Jie Zhang,*[a] Jinhua Piao[b] and Zhiyong Fu*[a]

a. The Key Lab of Fuel Cell Technology of Guangdong Province, Guangdong, School of Chemistry and Chemical Engineering, South China University of Technology, Guangzhou, 510640, China.

b. School of Light Industry and Food, South China University of Technology, Guangzhou, 510640, China.

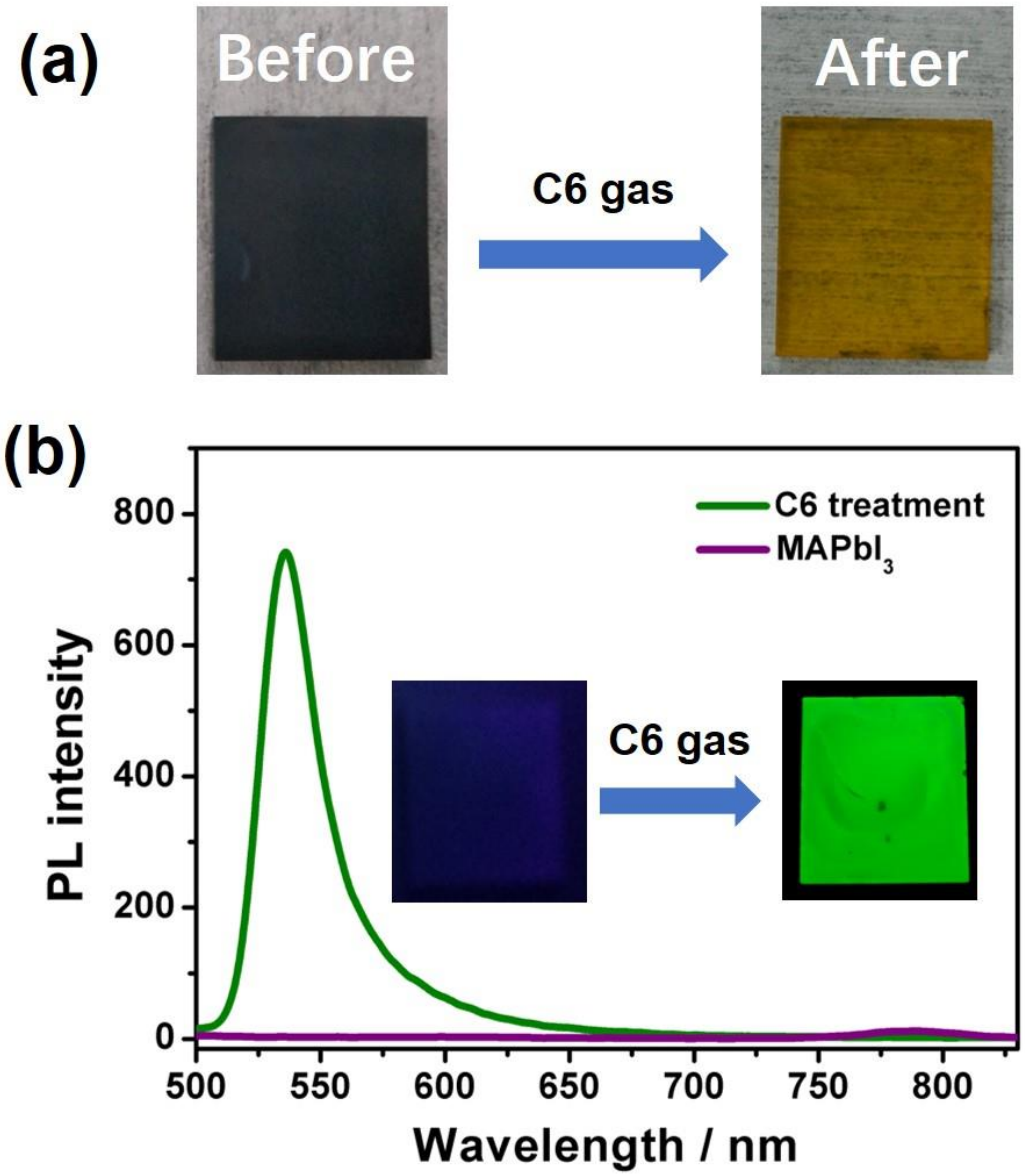

Fig. S1 (a) Photographs and (b) Photoluminescence spectra and fluorescent color of $MAPbI_3$ before and after the gaseous C6 treatment upon UV light (365 nm) irradiation.

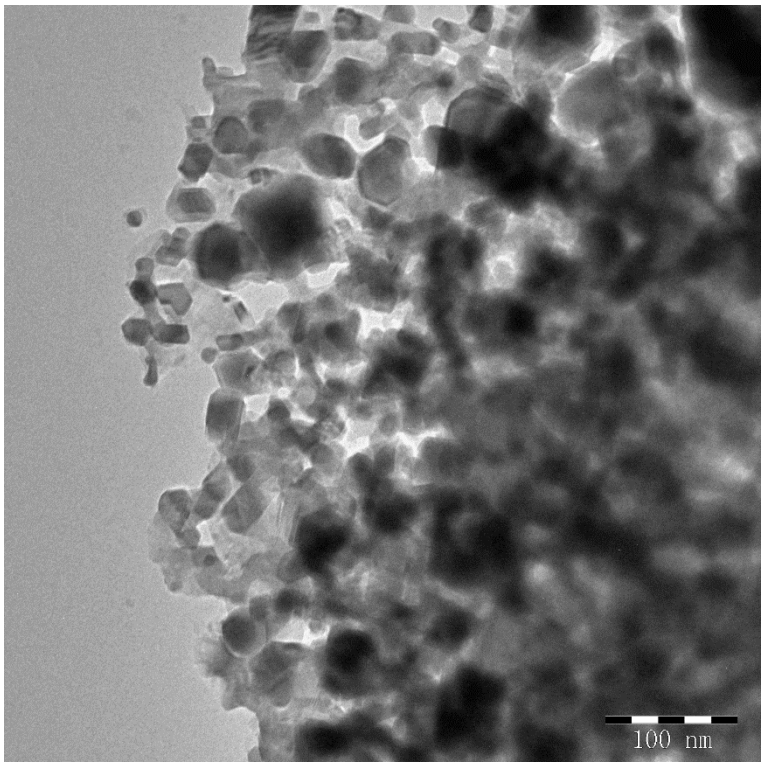

Fig. S2 TEM image of the 3D $MAPbI_3$ perovskite.

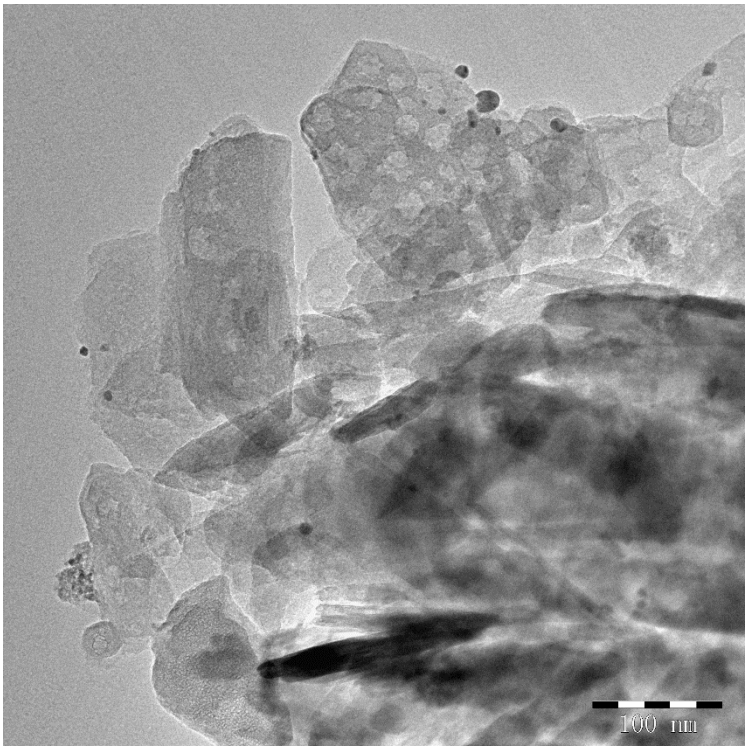

Fig. S3 TEM image of the 2D $(CH_3(CH_2)_5NH_3)_2PbI_4$ perovskite.

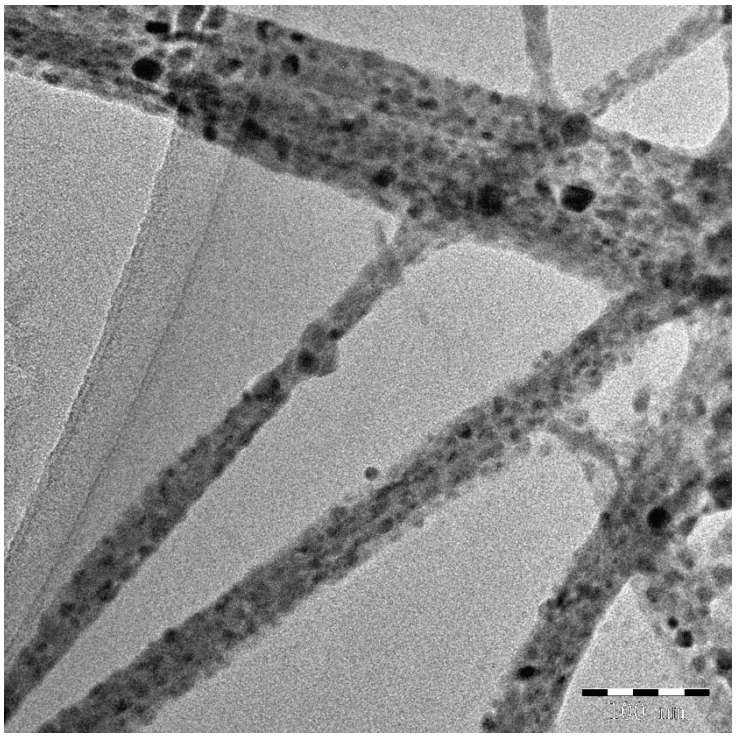

Fig. S4 TEM image of the 1D $(C_6H_{15}NH)PbI_3$ perovskite.

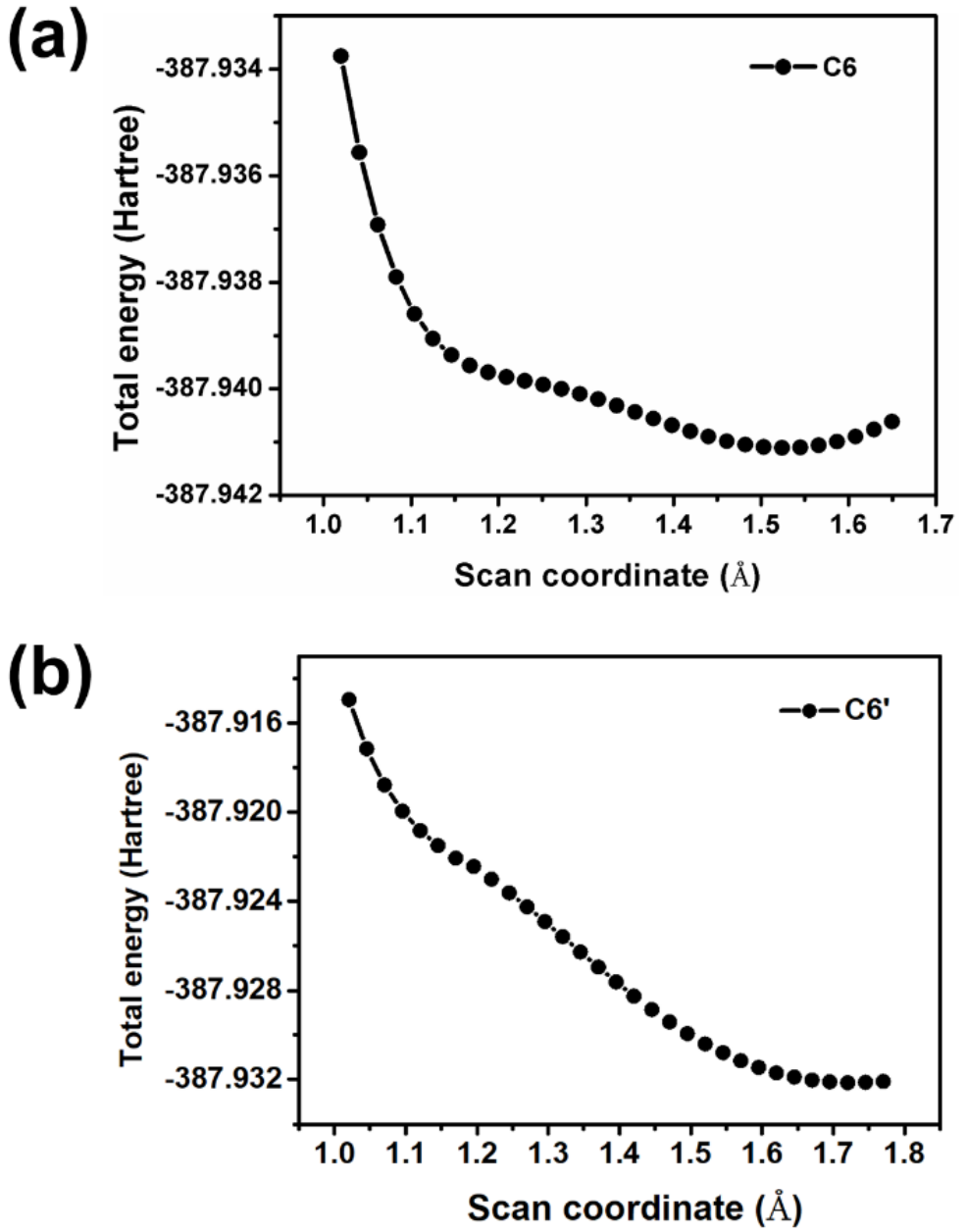

Fig. S5 Potential energy scan curve of proton transfer (a) from $CH_3NH_3^+$ to $CH_3(CH_2)_5NH_3^+$ (C6); (b) from $CH_3NH_3^+$ to $(CH_3CH_2)_3NH^+$ (C6').

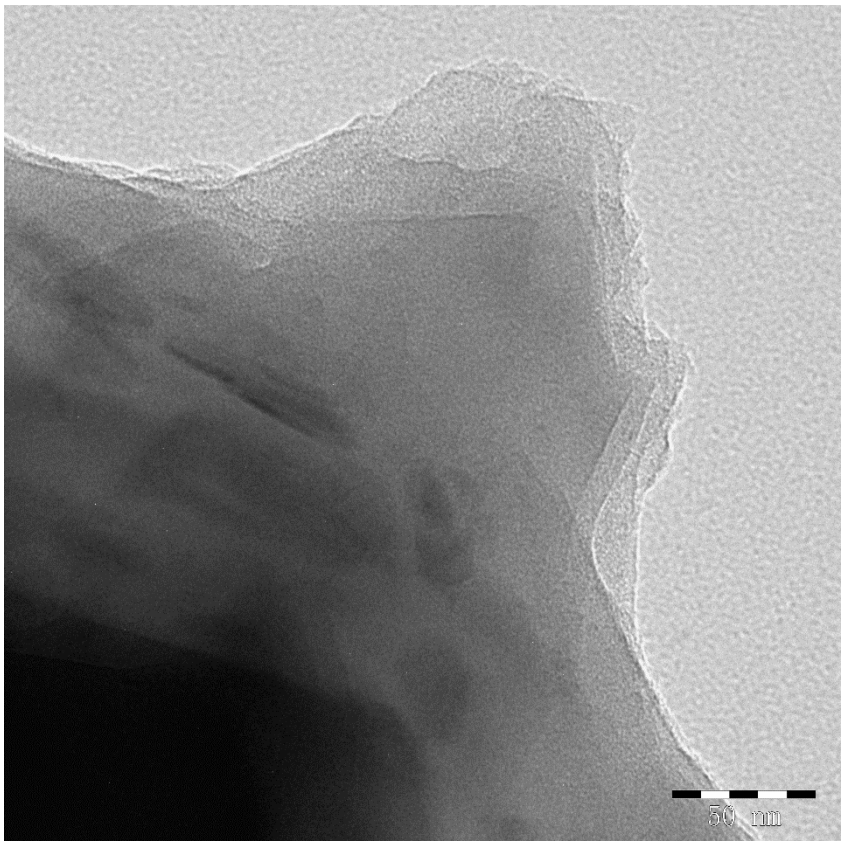

Fig. S6 TEM image of the quasi-2D perovskite.

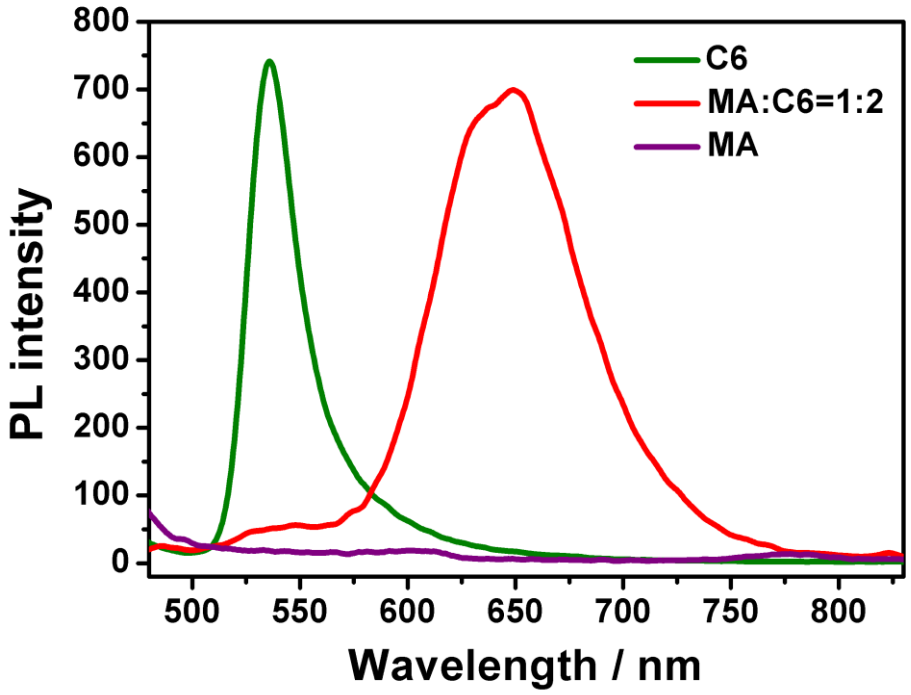

Fig. S7 Photoluminescence spectra for the transformed perovskite films from 3D $MAPbI_3$ with different ratios of mixed amines (MA/ C6).

DFT computations for the Optimized Structures

Cartesian Coordinates (Å), Free Energies at 298.15 K and 1 atm

CH_3NH_2

G = -95.801136 Hartree

N	-0.747205	-0.000009	-0.120699
H	-1.149025	0.812928	0.328293
H	-1.149079	-0.812922	0.328289
C	0.705460	-0.000011	0.017822
H	1.071443	-0.001061	1.050984

H	1.112292	-0.876783	-0.485758
H	1.112047	0.877964	-0.483848

$CH_3NH_3^+$

G = -96.139183 Hartree

N	0.706943	-0.000001	-0.000001
H	1.080785	0.160397	-0.939340
H	1.080755	-0.893716	0.330777
H	1.080736	0.733330	0.608579
C	-0.796574	0.000002	-0.000004
H	-1.137155	-0.795892	-0.655368
H	-1.137128	-0.169624	1.016961
H	-1.137150	0.965502	-0.361576

$CH_3(CH_2)_5NH_2$

G = -292.207557 Hartree

C	0.019271	0.484859	-0.000023
H	0.022005	1.142915	-0.875686
H	0.021998	1.142998	0.875579
C	1.287416	-0.359368	0.000022
H	1.291855	-1.015629	0.877421
H	1.291853	-1.015717	-0.877313
C	2.561261	0.480373	-0.000024
H	2.562252	1.137389	-0.873970

H	2.562267	1.137461	0.873866
N	3.813736	-0.266732	0.000008
H	3.863457	-0.869704	-0.813020
H	3.863618	-0.869354	0.813284
C	-1.257722	-0.346041	0.000012
H	-1.262134	-1.004217	-0.875632
H	-1.262140	-1.004136	0.875716
C	-2.525926	0.498678	-0.000031
H	-2.519705	1.155115	-0.875162
H	-2.519709	1.155198	0.875037
C	-3.793849	-0.345482	0.000007
H	-3.832087	-0.989141	0.881012
H	-4.690304	0.275058	-0.000026
H	-3.832082	-0.989228	-0.880935

$CH_3(CH_2)_5NH_3^+$

G = -292.555279 Hartree

C	0.054661	0.505045	-0.000009
H	0.053044	1.157848	0.878019
H	0.053043	1.157816	-0.878061
C	-1.213005	-0.348334	0.000007
H	-1.215538	-0.996289	-0.882520
H	-1.215537	-0.996258	0.882557

C	-2.450701	0.522596	-0.000007
H	-2.513828	1.151794	-0.886553
H	-2.513825	1.151826	0.886516
H	-3.719030	-0.943451	0.824407
H	-4.556175	0.222833	0.000001
H	-3.719033	-0.943479	-0.824367
N	-3.700464	-0.337412	0.000010
C	1.320278	-0.344775	0.000005
H	1.318693	-0.999870	0.877178
H	1.318692	-0.999902	-0.877144
C	2.590985	0.497061	-0.000011
H	2.588271	1.151744	-0.875959
H	2.588272	1.151776	0.875912
C	3.850401	-0.358768	0.000003
H	3.886696	-1.000374	-0.881882
H	4.747094	0.259258	-0.000009
H	3.886698	-1.000342	0.881911

$N(CH_2CH_3)_3$

G = -292.193095 Hartree

N	-0.000078	-0.000053	-0.171818
C	-1.386284	0.086855	0.274423
C	-2.269808	-1.042262	-0.236489

H	-1.793971	1.026327	-0.095880
H	-1.436197	0.128892	1.378493
H	-3.318033	-0.788109	-0.078065
H	-2.108816	-1.188391	-1.305685
H	-2.083636	-1.986213	0.273915
C	0.617828	-1.244040	0.274439
C	2.037666	-1.444378	-0.235889
H	0.008243	-2.066842	-0.096105
H	0.606149	-1.308495	1.378502
H	2.341738	-2.479231	-0.077468
H	2.084280	-1.231666	-1.305005
H	2.761647	-0.811157	0.275070
C	0.768488	1.157056	0.273992
C	0.232124	2.486785	-0.236551
H	1.785698	1.040331	-0.096958
H	0.830647	1.179347	1.378018
H	0.976576	3.267416	-0.078821
H	0.024064	2.420417	-1.305545
H	-0.677916	2.797649	0.274700

$NH(CH_2CH_3)_3^+$

G = -292.561733 Hartree

H	-0.000325	0.000183	-1.208873

N	-0.000104	0.000022	-0.184677
C	-1.352842	0.498378	0.256654
C	-2.497448	-0.397670	-0.171299
H	-1.467063	1.488373	-0.176785
H	-1.293824	0.601976	1.340977
H	-3.429739	0.135422	0.008505
H	-2.452547	-0.623843	-1.238552
H	-2.539176	-1.328450	0.389508
C	0.244627	-1.420900	0.256022
C	1.593327	-1.963805	-0.171024
H	-0.555251	-2.014647	-0.178321
H	0.124562	-1.422171	1.340243
H	1.597403	-3.037942	0.007622
H	1.768185	-1.810659	-1.237865
H	2.419616	-1.535352	0.391341
C	1.108119	0.922283	0.256209
C	0.904293	2.361680	-0.171205
H	2.022329	0.526266	-0.177833
H	1.169022	0.819111	1.340462
H	1.832352	2.902301	0.008052
H	0.685107	2.436275	-1.238241
H	0.119626	2.863209	0.390368