Surface structure of quasi-2D perovskite

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Introducing a small amount of large organic cations (e.g. PEA, BA and AVA) in 3D perovskite (e.g. $CH_3NH_3PbI_3$) forms quasi-2D perovskite and significantly enhances the stability of the perovskite solar cell against moisture and light.[1] After a large organic cation is replaced with a small organic cation, possible structures may form as shown in Figure 1. Whereas the 2D perovskite with small number of layers is established to take the Ruddlesden–Popper (RP) phase, the structure of the quasi-2D perovskite with a thick perovskite layer has never been proved.

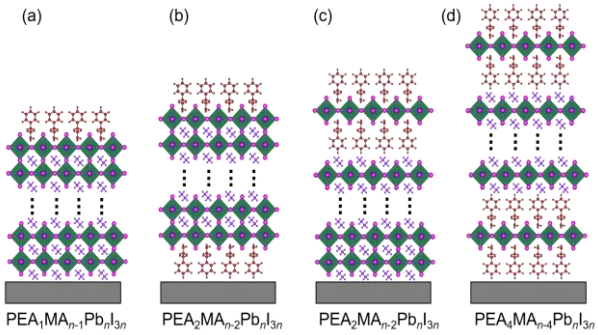

Fig.1 Possible structures of the qusai-2D perovskite

In this work, we investigate the surface structure of the quasi-2D perovskites with R= $C_6H_5CH_3CH_2NH_3$ (PEA), A= CH_3NH_3, B= Pb and X= I. Recently we examined surface termination of solution processed $MAPbI_3$ film using ultraviolet photoelectron spectroscopy (UPS) and metastable-atom electron spectroscopy (MAES).[2] UPS examines the valence electronic states of materials based on the photoemission excited by ultraviolet photons. In MAES, excitation source is replaced with metastable He atom. MAES selectively sensitive to the outermost surface atoms because the metastable atoms do not penetrate into the inner layers.[3] Therefore, combination of the UPS and MAES enables us to obtain the information about the outermost surface.

We proved that PEA ligands cover the surface of 3D perovskite in both cases. From the dependence of concentration of PEAI in the precursor solution, we gain more precise structural information. We found that 0.5 % of PEA is insufficient to cover the 3D surface and the increased PEA ratios of 5 %, 10 % and 20 % fully covered the surface. 1 % PEA is the intermediate case and just sufficient to cover the 3D surface. These results indicate that, the plausible structure of the quasi-2D perovskite is shown in Figure 1.d that 2D perovskite layers covered the surface and bottom of the 3D perovskite.

References

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