Efficient and stable Ruddlesden—Popper perovskite solar cells with unique interlayer molecular interaction

With the support by the National Natural Science Foundation of China, the research team led by Prof. Chen YongHua (陈永华) from the Institute of Advanced Materials (IAM), Nanjing Tech University (Nanjing Tech), proposed a strategy for building efficient and stable layered perovskite solar cells based on heteroatom organic mines, which was published in *Nature Photonics* (2020, 4: 154—163).

Perovskite materials have attracted much attention in recent years because of their excellent optoelectronic properties for solar cells, including high optical absorption, small exciton binding energy, low trap densities, and long-range ambipolar carrier diffusion lengths. However, perovskite materials are easily degraded under the conditions of light, electric field, heating, water and oxygen, which seriously hinder the further commercialization of perovskite solar cells (PSCs). Compared to the traditional three-dimensional (3D) halide perovskite, the two-dimensional Ruddlesden—Popper (2DRP) layered perovskite greatly enhances the light and thermal stability of perovskite, due to moisture resistance, ultra-low self-doping to prevent unintentional defects, and reduced ion mobility. The stability of the 2DRP layered perovskite framework originates from the Van der Waals forces between two organic amine molecules. However, weak van der Waals forces limit the improvement of stability and hinder the self-assembly of 2DRP layered perovskites. Therefore, the interaction between the organic amine molecules is the key to improve stability and efficiency of 2DRP PSCs.

Chen's group innovatively introduced an organic amine molecule containing sulfur (S) atom, 2-(methylthio) ethylamine hydrochloride (MTEACl), to construct 2DRP perovskite $(MTEA)_2(MA)_{n-1}Pb_nI_{3n+1}$. The additional sulfur—sulfur (S—S) interaction between the S atoms in the two MTEA molecules was observed as compared to traditional 2DRP perovskite $(BA)_2(MA)_{n-1}Pb_nI_{3n+1}$ (BA: butylamine). The S—S interaction enables strong out-of-plane preferential growth of perovskite crystals, which greatly improves charge transport and reduces trap density. Therefore, a high-performance 2DRP PSC with a PCE as high as 18.06% was achieved with the certification efficiency of 17.80% from the National Institute of Metrology in China, which is one of the best reported efficiencies. Most importantly, this strategy greatly stabilized the layered perovskite framework, leading to the improved moisture, thermal, and light stability of the perovskite films and devices. The efficiency decay is less than 15% under operational conditions at the maximum power point for 1 000 h under continuous 1 sun, AM1.5G illumination. This work provides an alternative opportunity to tailor this scientifically and technologically interesting class of hybrid perovskites for potential applications.

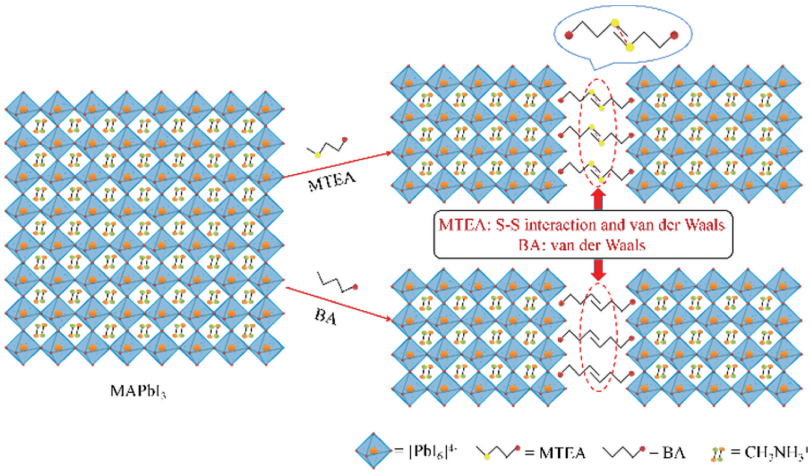

Figure Schematic crystal structures and interactions of the 2DRP perovskites $(MTEA)_2(MA)_{n-1}Pb_nI_{3n+1}$ and $(BA)_2(MA)_{n-1}Pb_nI_{3n+1}$.