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Interactions between 2D Halide Perovskite Materials and Methylamine

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Introduction

The structural tunability of halide perovskites, shown below, offers exciting potential for their use as photovoltaic materials and as semiconductors in diverse applications. We investigate 2-dimensional Ruddlesden-Popper (RP) phase halide perovskite structural stability by the intercalation-deintercalation of methylamine gas.

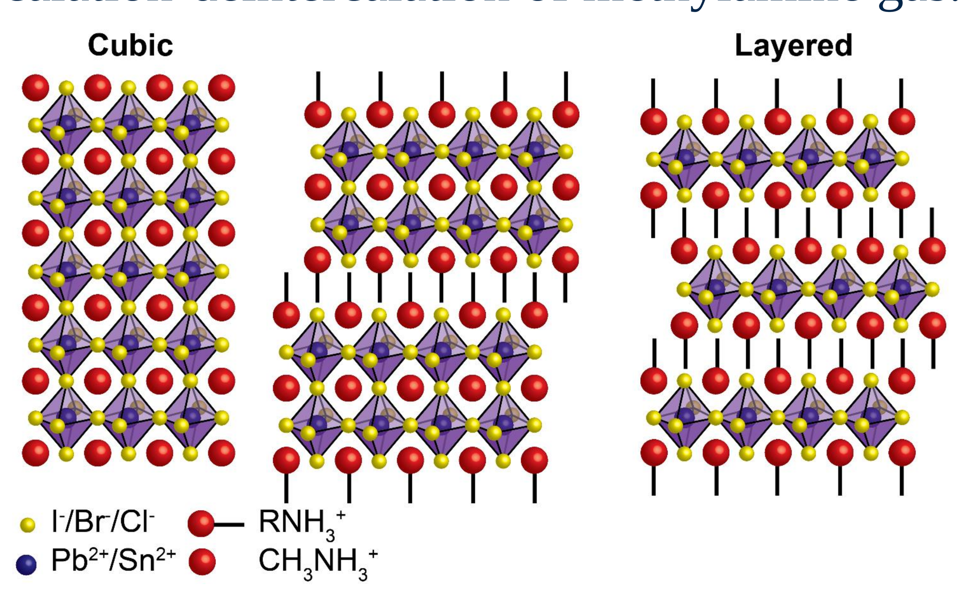

Figure. Structure of the 3D ABX_3 halide perovskites shown at left. A 2D Ruddlesden-Popper phase perovskite shown at right along with an intermediate 2D/3D phase (center).

Switchable Windows[1]

- Photo-thermal heating can lead to switchable $MAPbI_3$ solar cells in the presence of MA gas
- Switchable PV circumvents the fundamental efficiency-transparency tradeoff of PV windows
- Morphological changes lead to degradation

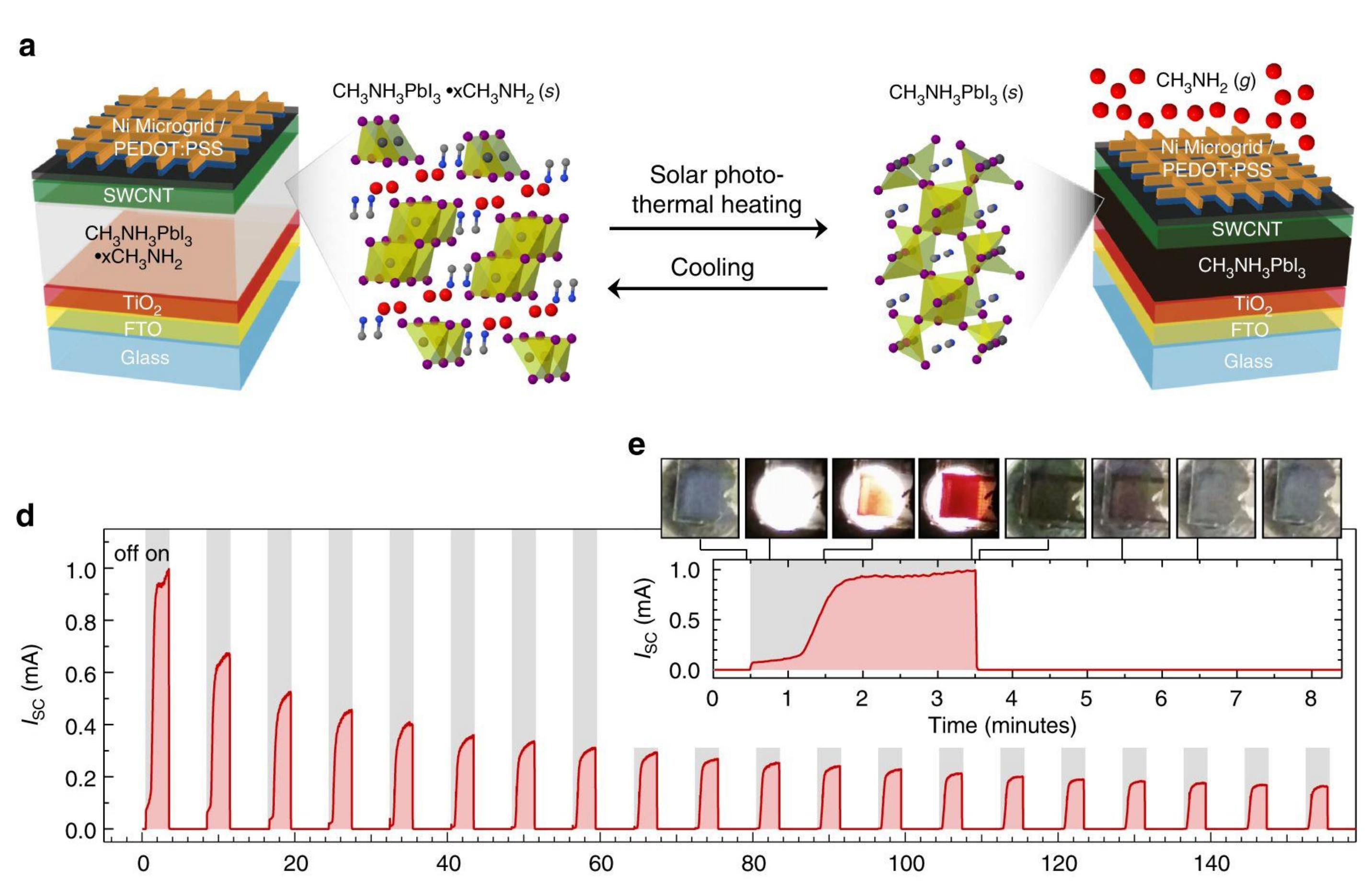

Figure. Schematic of switchable PV window operation (top). Photocurrent of devices with time for 20 switches (bottom). From Reference 1.

Project Goal: Evaluate interactions between A-site organic spacers and lead halide sheets in 2D perovskites.

Experiment

- Expose A_2PbI_4 films to MA vapor to form intercalation compound
- Remove MA to deintercalate

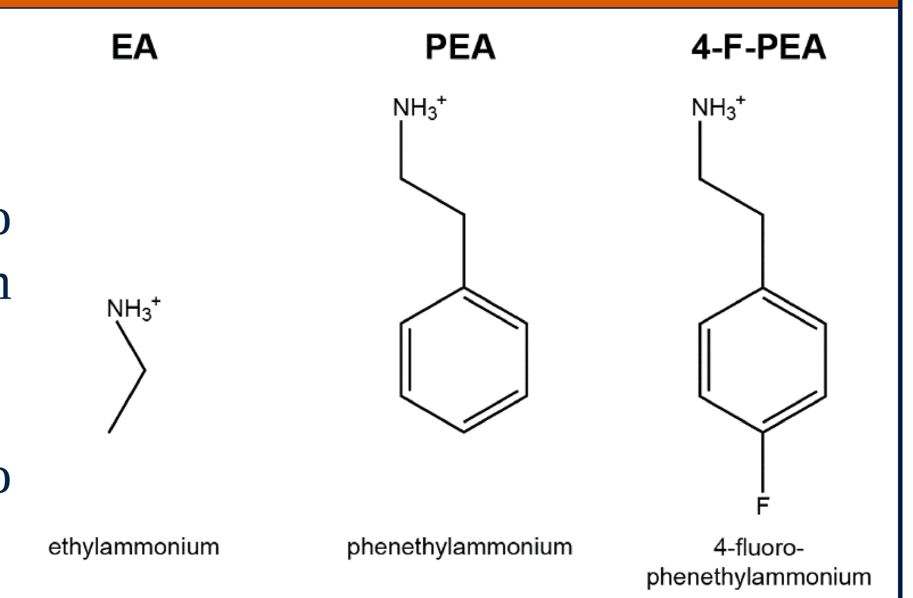

Figure. Chemical structure of A-site organic cations used in this work.

Key Findings:

- Incorporation of MA in PEA_2PbI_4 and 4-F-PEA_2PbI_4 forms stable $A_2MA_1Pb_2I_7$
- $MAPbI_3$ phases appear to form initially EA_2PbI_4 materials after MA exposure

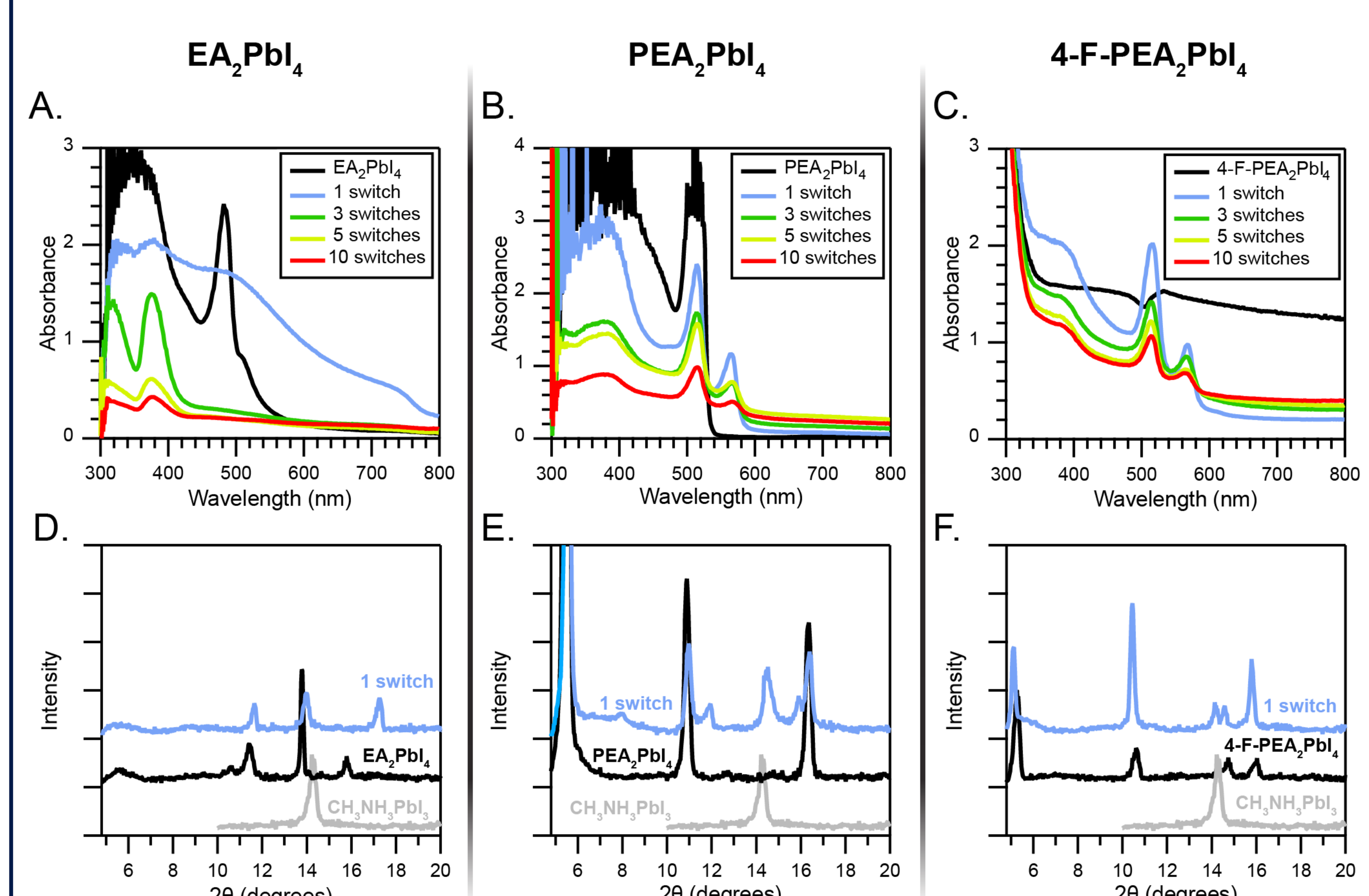

Figure. A)-C) UV-visible absorption spectra of EA_2PbI_4, PEA_2PbI_4, and 4-F-PEA_2PbI_4 films, respectively. Black traces show the as-synthesized films. Colored traces show the absorption properties of the films following 1 to 10 brief exposures to MA gas (*i.e.*, switches). D)-F) Power XRD patterns of EA_2PbI_4, PEA_2PbI_4, and 4-F-PEA_2PbI_4 films, respectively, before (black) and after (blue) one switch with MA gas, offset for clarity. The XRD pattern of a $MAPbI_3$ film (grey) is shown for comparison.

Improved Stability[2]

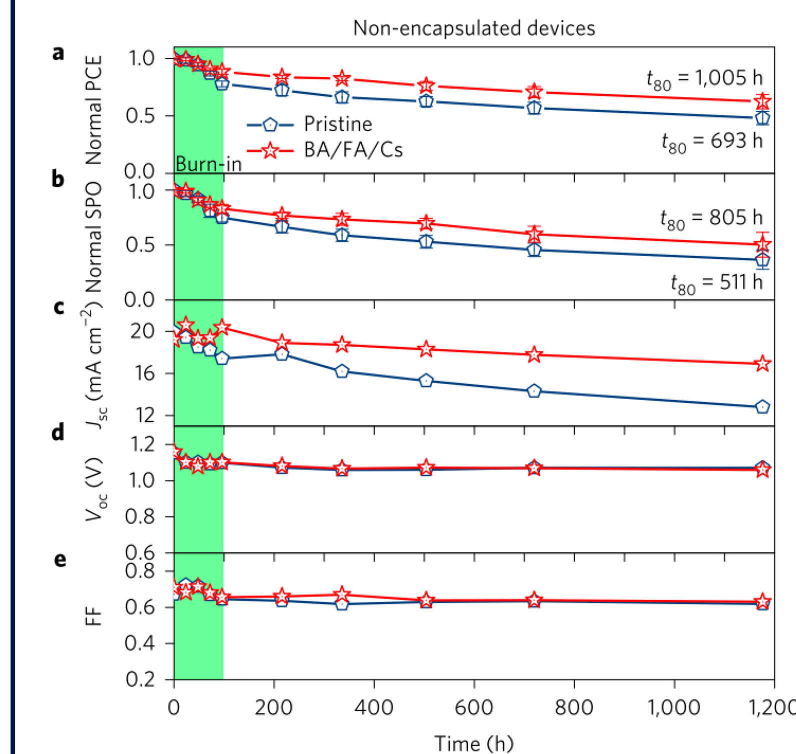

Figure. Operational stability comparison of 3D (blue) and mixed 2D/3D halide perovskite solar cells. From Reference 2.

- Stability gains realized for mixed 2D/3D materials
- Can reduce moisture sensitivity
- Improvement mechanism still unclear

Conclusions

- n = 2 materials preferentially formed (vs. n=1 or n>2) upon MA exposure
- Yields insight into hierarchical structures in some mixed 2D/3D perovskites (regions of 3D and low dimensionality materials).[3]
- Exploration of other A-site cations to improved design rules for mixed 2D/3D halide perovskites

References

1. Wheeler, L. M. *et al. Nat. Commun.* **2017**, *8* (1), 1722.
2. Wang, Z.; Lin, Q.; Chmiel, F. P.; Sakai, N.; Herz, L. M.; Snaith, H. J. *Nat. Energy* **2017**, *6* (August), 17135.
3. G. Grancini et al., *Nat. Commun.* **2017**, 8 (June), 1–8.

Acknowledgements

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