GMF
Group for Molecular Engineering of Functional Materials

2D Perovskite as a Hole Transporting Material for Efficient and Stable Perovskite Solar Cells

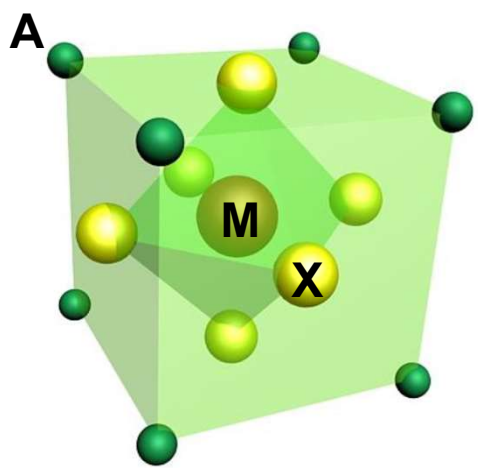
Hobeom Kim

30. 09. 2019

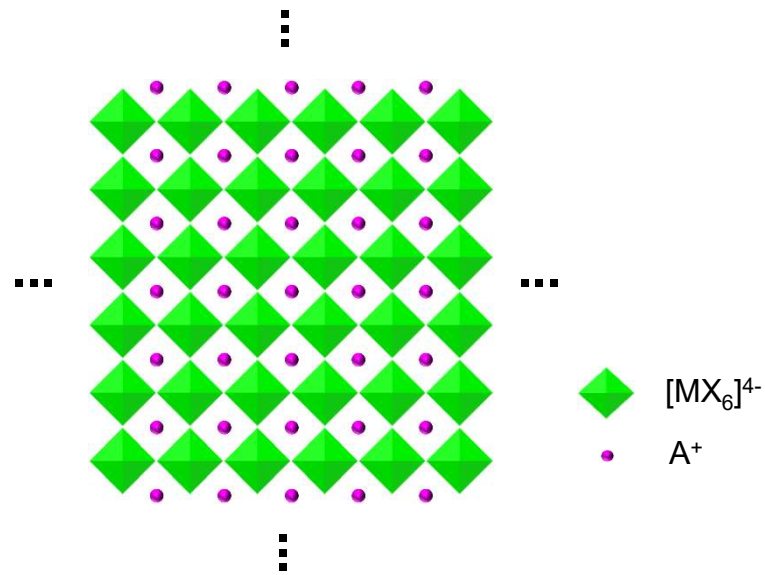
EPFL

Metal-Halide Perovskite

Unit Cell of Metal-Halide Perovskite



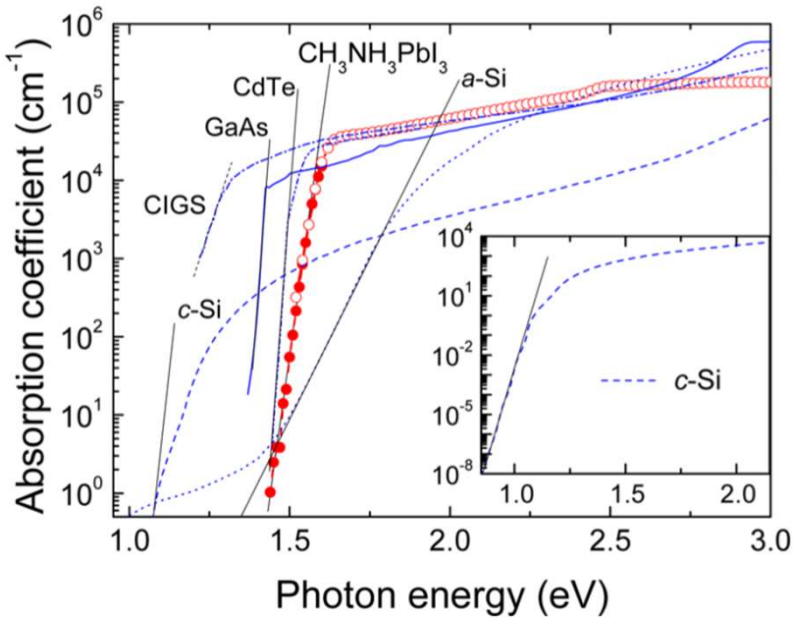
Crystal Structure of Metal-Halide Perovskite

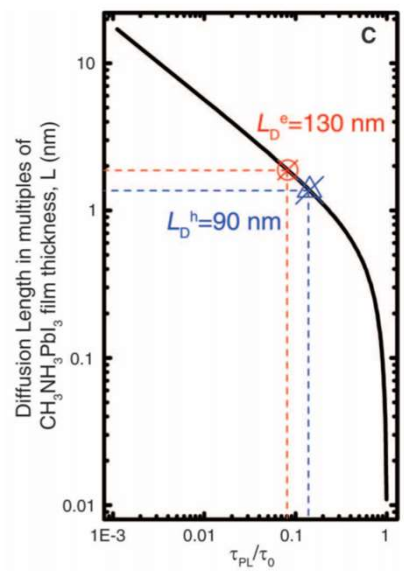


AMX_3

A: Organic Ammonium or Alkali Metal (Cs, Rb and K)
M: Metal (Pb, Sn)
X: Halide (I, Br, Cl)

Perovskite as a Light Absorber

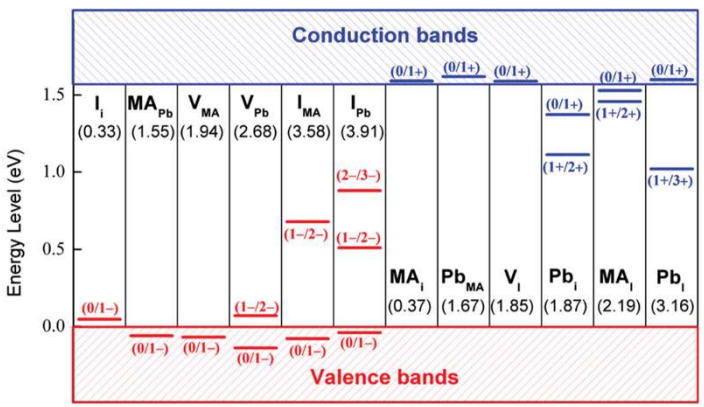


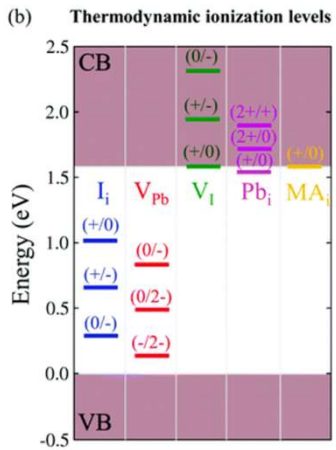


C. Ballif et al., *J. Phys. Chem. Lett.*, 5, 1035 (2014)
T. C. Sum et al., *Science*, 342, 344 (2013)

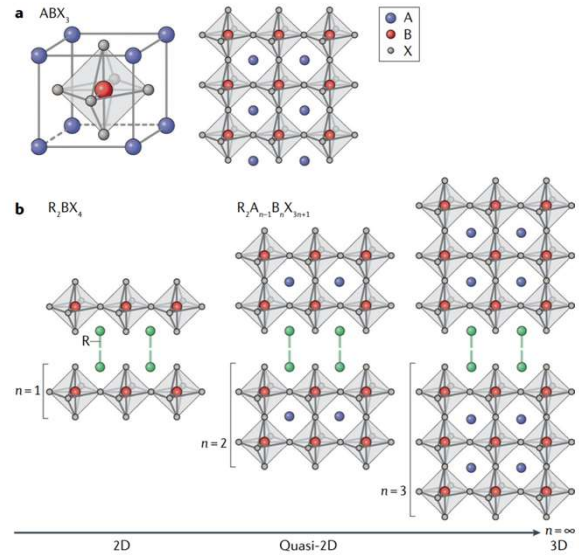
- ✓ Broad absorption.
- ✓ High absorption coefficient
- ✓ Long diffusion length
- ✓ High mobility of charge carriers

Limitation in 3D Perovskites



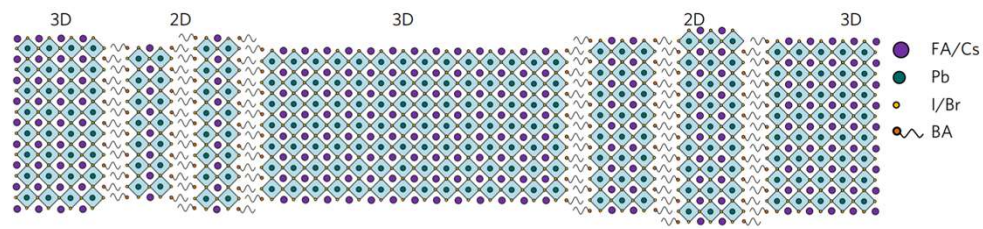


Y. Yan et al., *Adv. Mater.*, 26, 4653 (2014)
A. Petrozza and F. Angelis et al., *Energy Environ. Sci.*, 11, 702 (2018)



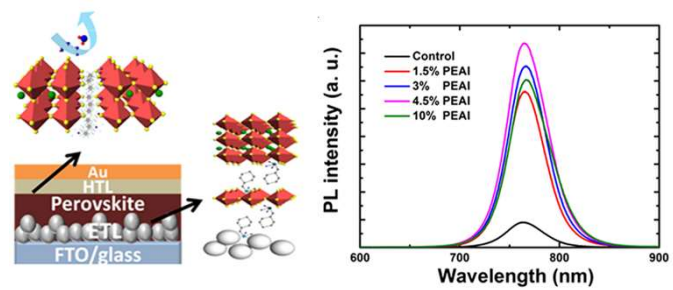
M. K. Nazeeruddin et al., *Nature Rev. Mater.*, 4, 4 (2019)

- ✓ Defects and trap states
  - → Non-radiative recombination
  - → Degradation of device efficiency



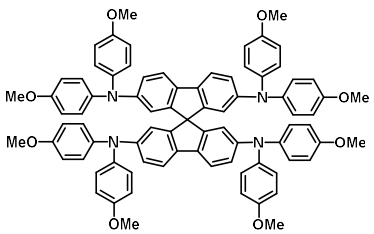
H. Snaith et al., *Nature Energy, 2*, 17135 (2017)

- ✓ ***Incorporation of 2D perovskite can lead to passivation of defect and reduction of density of trap states.***

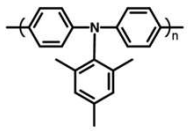


A. Ho-Baillie et al., *ACS Energy Lett.*, 3, 647 (2018)

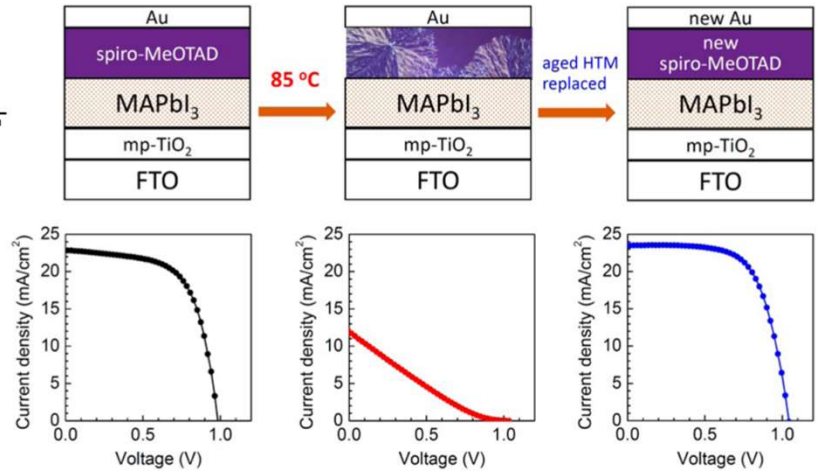
Limitation in Organic HTMs

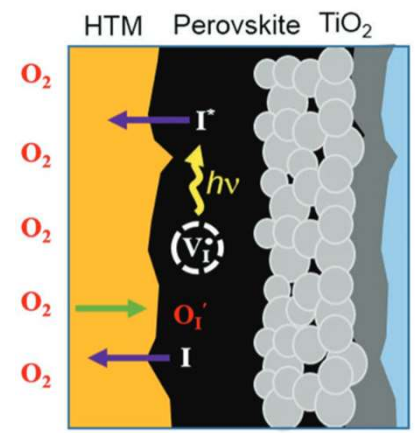


Spiro-OMeTAD



PTAA





N.-G. Park et al., *ACS Appl. Mater. Interfaces*, 9, 7148 (2017)
J. Seo et al., *Adv. Sci.*, 6, 1900528 (2019)

✓ Pros

- Good solubility
- Reasonably high hole mobility
- Easy processability
- Favourable energetic configuration

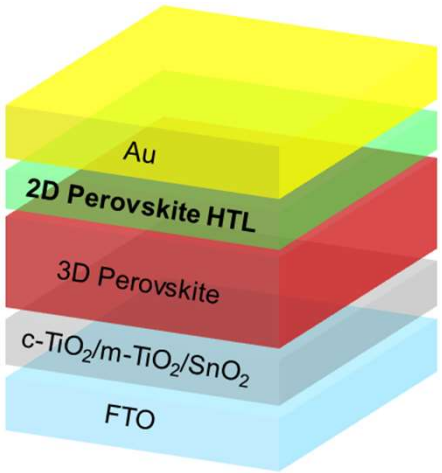
✓ Cons

- **Necessary to use dopants to improve charge mobility**
  → Degradation of devices
- **Hygroscopic dopant**
- **High cost**
- **Complex multi-step synthesis and purification processes**

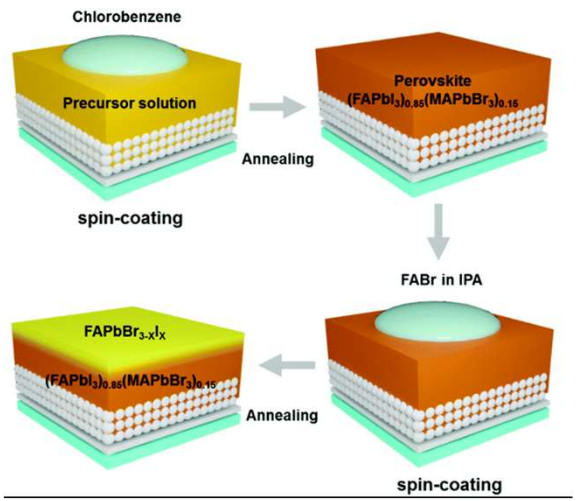
2D Perovskite as an HTL for Solar Cells

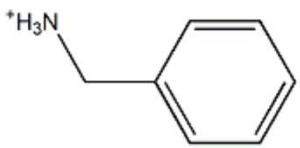
The dual role of the 2D perovskite

as an HTL and a passivation layer



$Cs_{0.08}FA_{0.77}MA_{0.12}PbI_{2.62}Br_{0.35}$



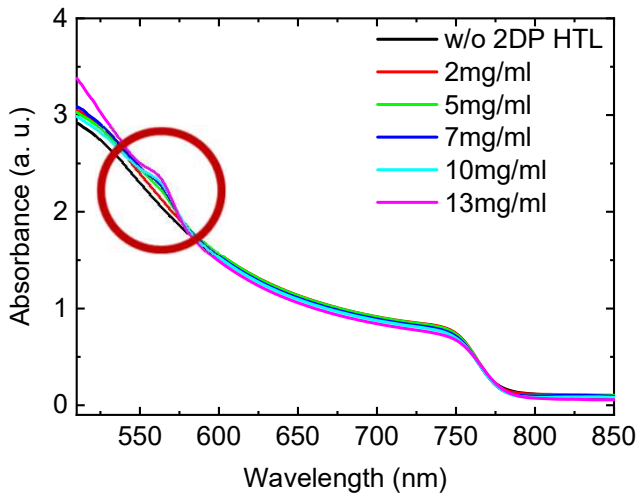


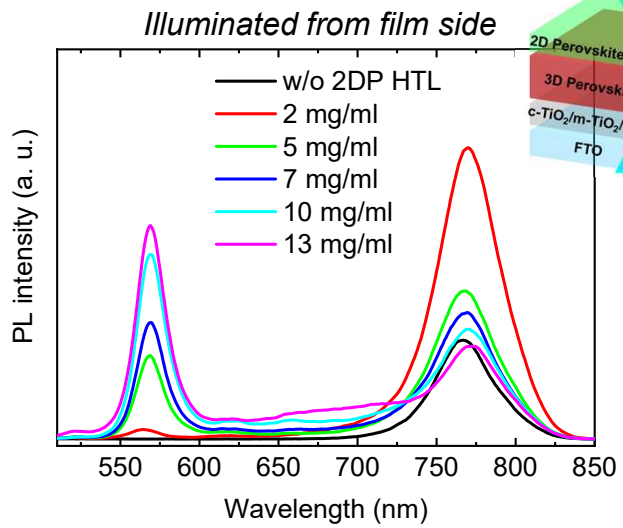
Benzylammonium iodide

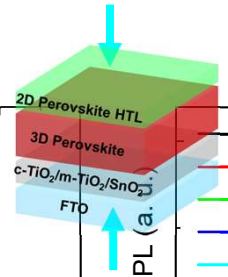
M. K. Nazeeruddin et al., *Energy Environ. Sci.*, 10, 621 (2017)

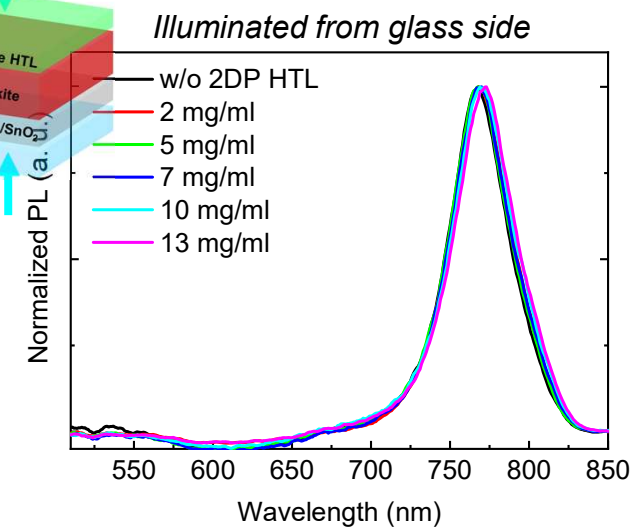
2D Perovskite as an HTL for Solar Cells

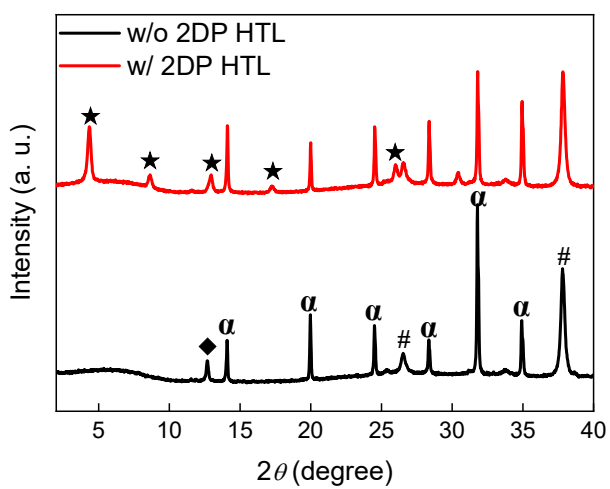
➢ Characterization of 2D Perovskite

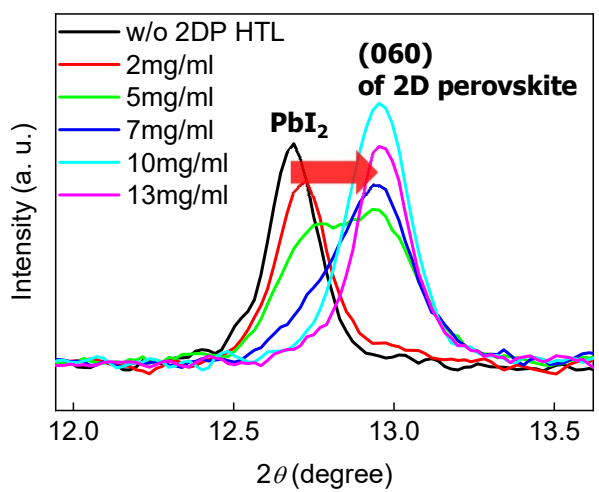












The formation of 2D perovskite was c onfirmed with various characterizatio ns.

$$2PbI_2 + 2BnA^+ + Z^+ + 3X^-$$

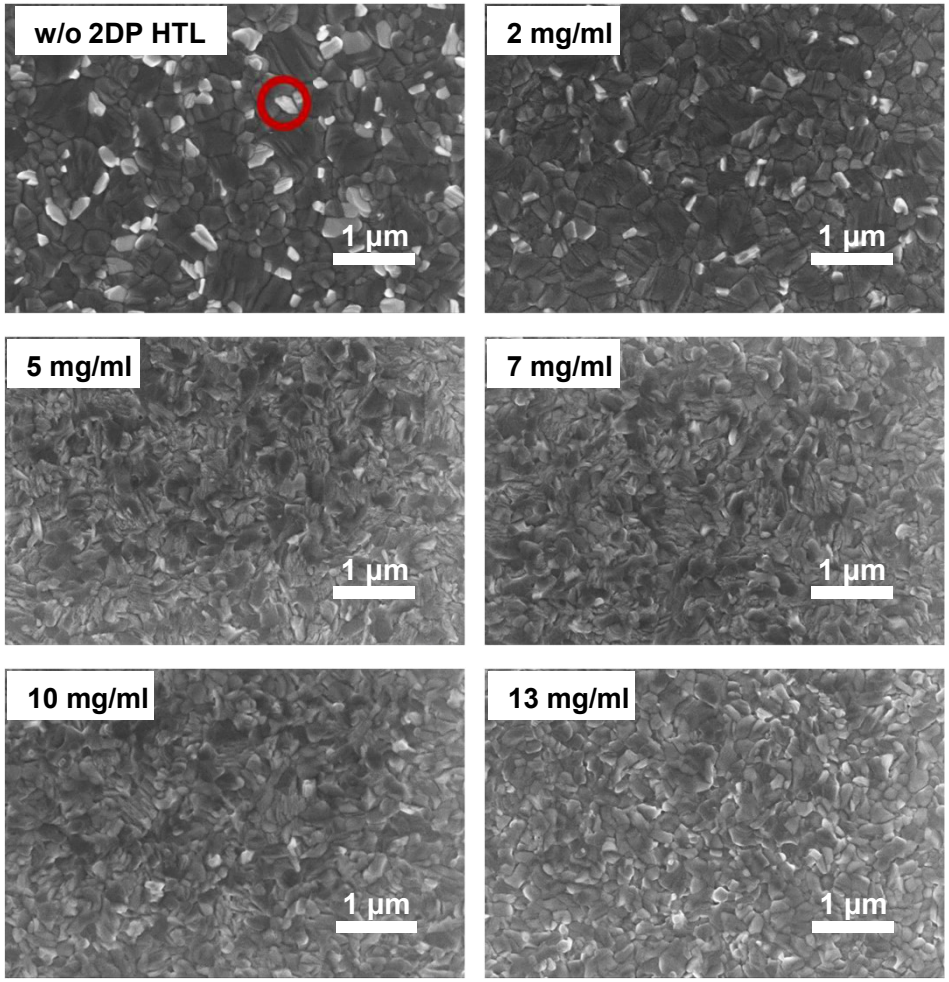
$$\rightarrow BnA_2ZPbX_7$$

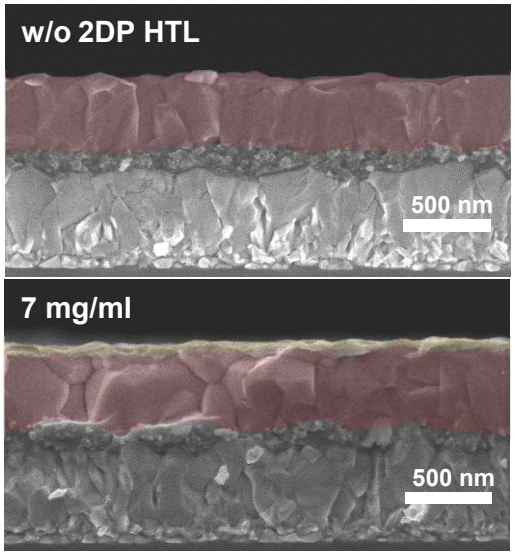
Z is a combination of FA, MA and Cs.

Under review

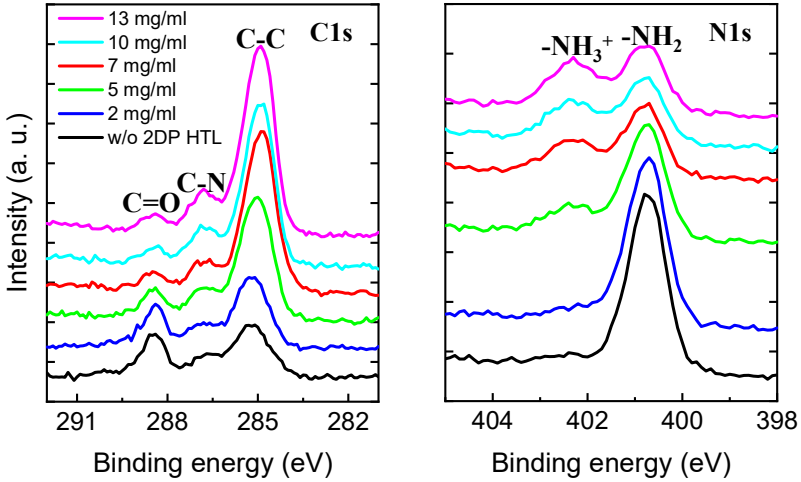
2D Perovskite as an HTL for Solar Cells

- Film morphology of perovskites





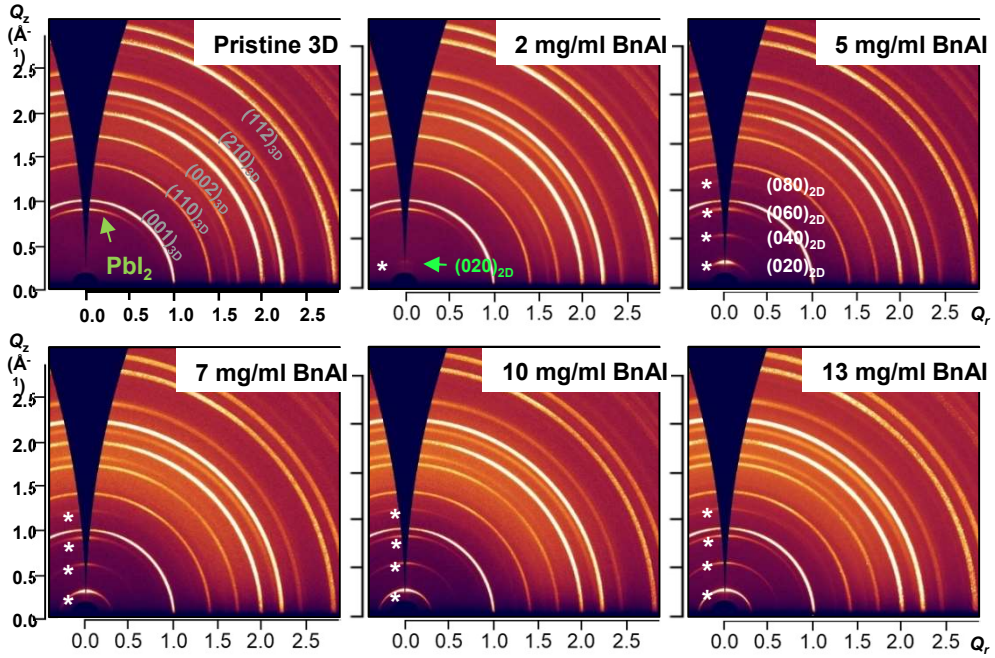
- Study on chemical bonds (XPS)

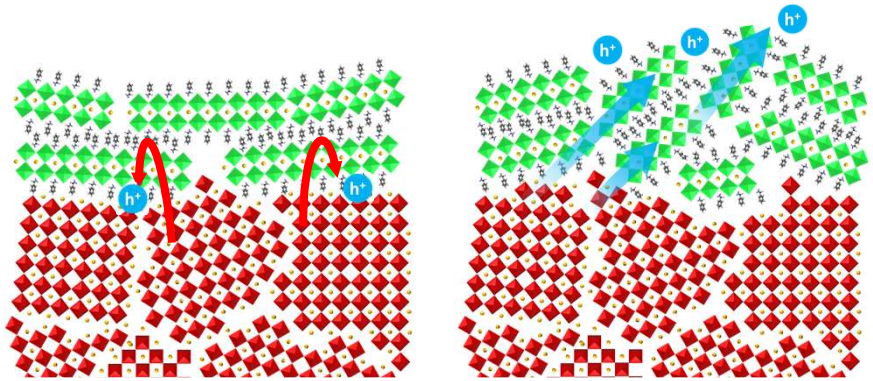


Under review

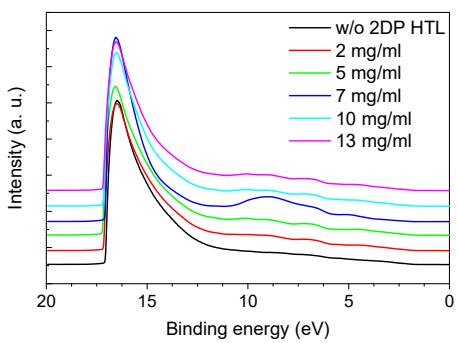
2D Perovskite as an HTL for Solar Cells

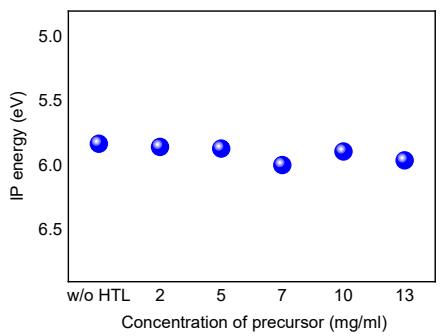
➢ Orientation of 2DP Perovskite (GIXD)



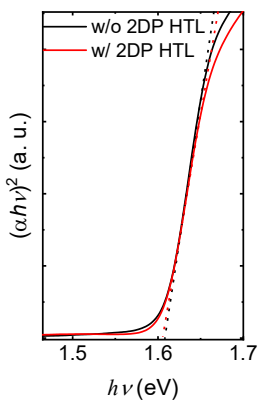


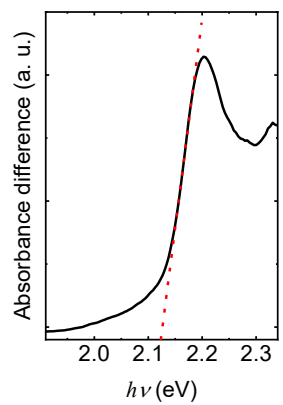
➢ UPS

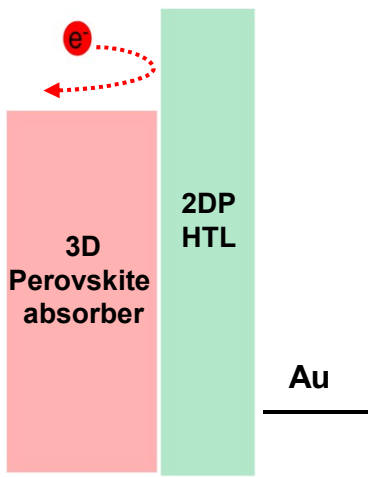




➢ Tauc-plot



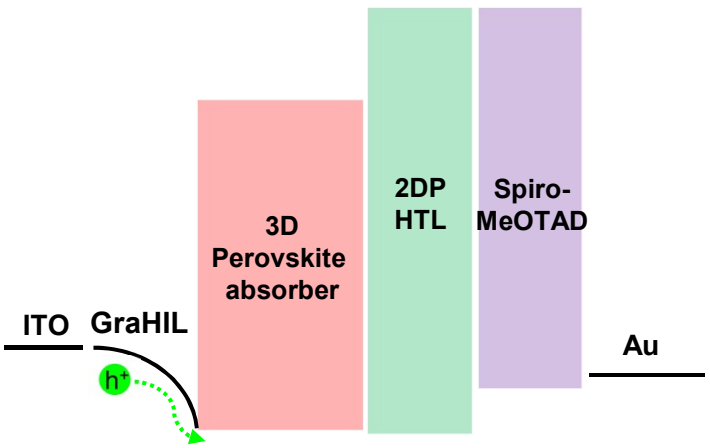


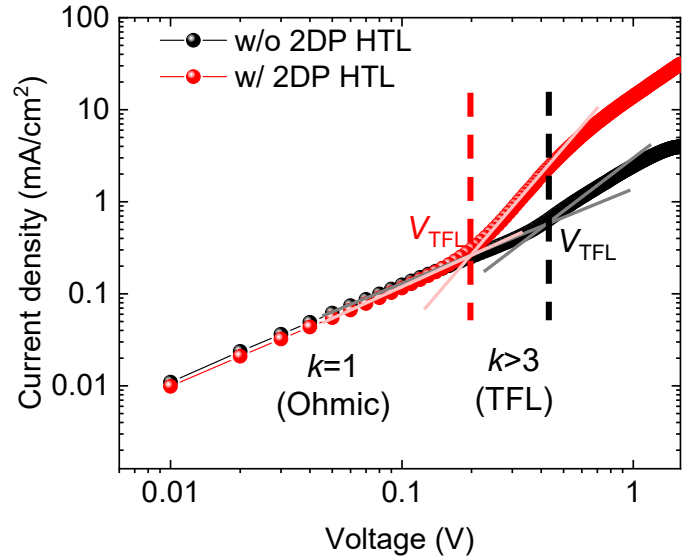


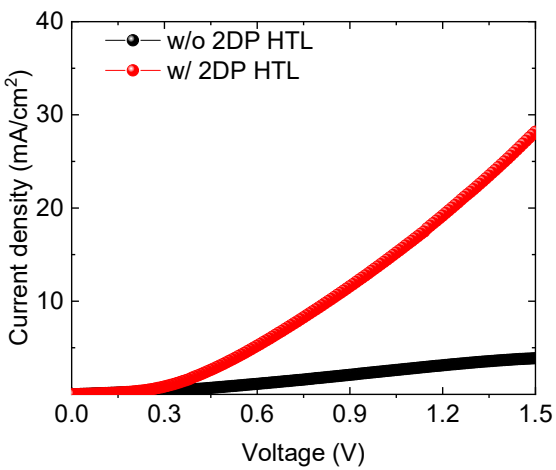
Under review

2D Perovskite as an HTL for Solar Cells

- Trap passivation and hole current (mobility)







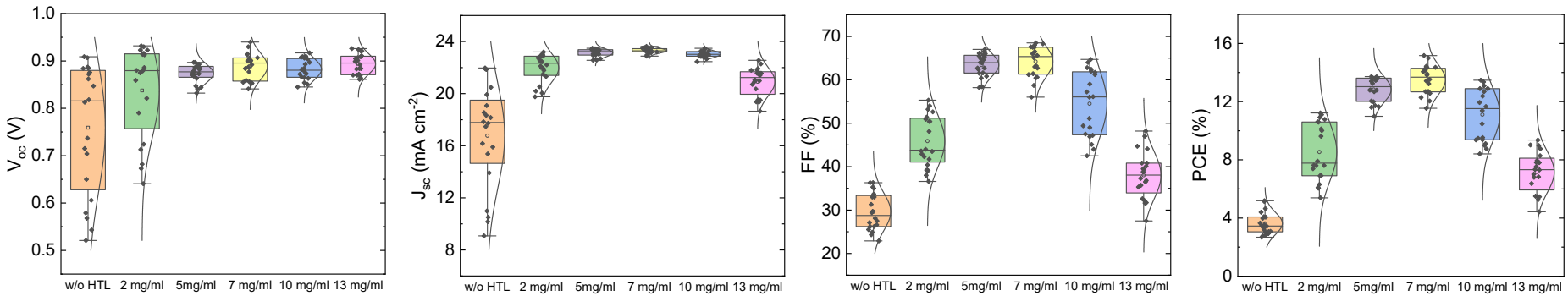
$$V_{\mathrm{TFL}} = n_{\mathrm{t}} \frac{eL^2}{2\varepsilon\varepsilon_0} \qquad J = \frac{9\varepsilon\varepsilon_0 \mu_h V^2}{8L^3}$$

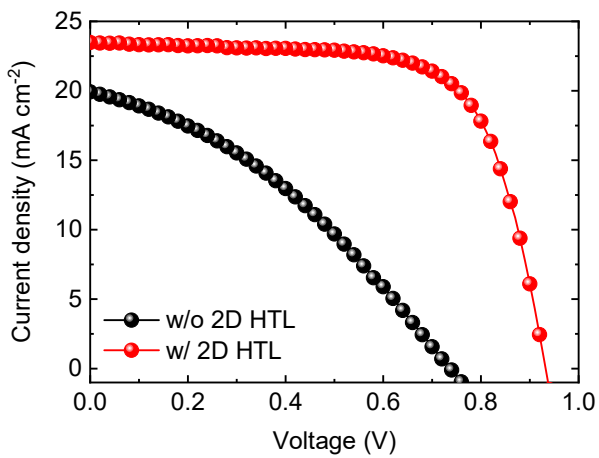
	V_{TFL}[V]	n_{t}[cm^{-3}]	μ_{h}[cm^2/V·s]
w/o 2DP HTL	0.418	6.02×10^{15}	0.1135
w/ 2DP HTL	0.198	2.43×10^{15}	0.6469

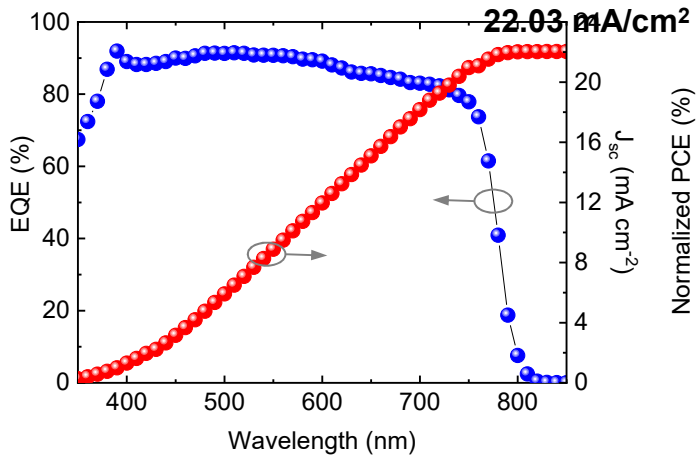
Under review

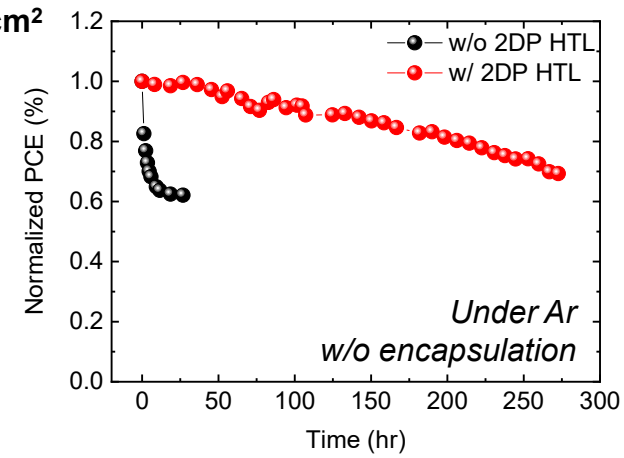
2D Perovskite as an HTL for Solar Cells

➢ Photovoltaic characteristics





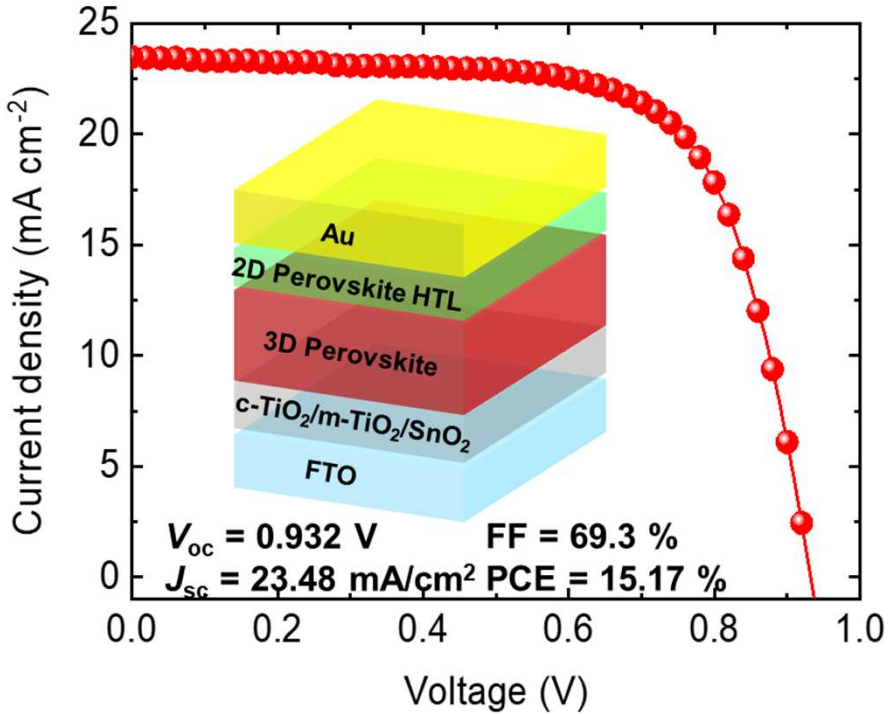




w/o 2DP HTL	***w/ 2DP HTL***
V_{oc} = 0.737 V	**V_{oc} = 0.932 V**
J_{sc} = 19.92 mA/cm^2	**J_{sc} = 23.48 mA/cm^2**
FF = 35.3 %	**FF = 69.3 %**
PCE = 5.19 %	**PCE = 15.17 %**

Under review

Conclusion



2D perovskite can function as an effective HTL and also a passivating layer.

The random orientation of the 2DP HTL can facilitate hole transport.

The 2DP HTL significantly increased PCE and extended the operational lifetime.

Acknowledgement

GMF
Group for Molecular Engineering of Functional Materials

Thank you for attention

EPFL

Group for Molecular Engineering of Functional Materials (GMF)

Apolo

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Mr. Mingyuan Pei