« Exchange of Experiences » - Webinar

Insights, outcomes and results – 28 September 2023

SCALEUP: Large scale molecular simulation of perovskite solar cells

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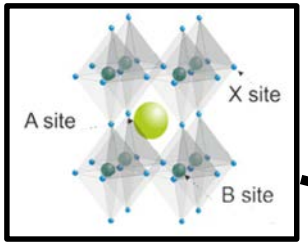
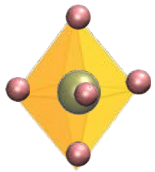
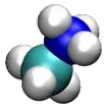
- Scientific & technical challenges addressed

Metal-halide Perovskite (MHP)s: ABX_3

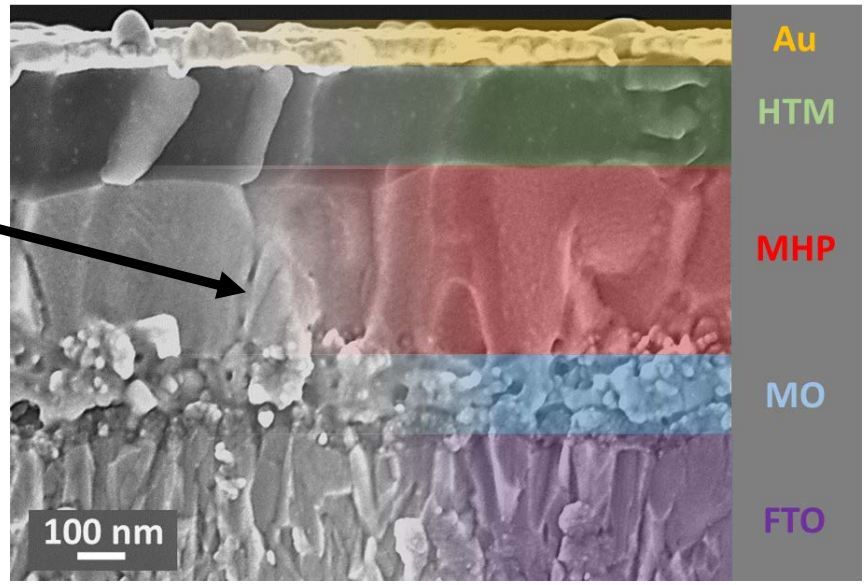




BX_6 octahedral units
(B = Pb, X= I,Br,Cl)



A^+
($A = CH_3NH_3^+$, FA^+ , Cs^+)



Metal-halide Perovskite (MHP)s: ABX_3

HTM = Spiro-OMeTAD, more stable alternative materials

MHP = multicompositional metal halide perovskites

MO = TiO_2, SnO_2

Long diffusion lengths

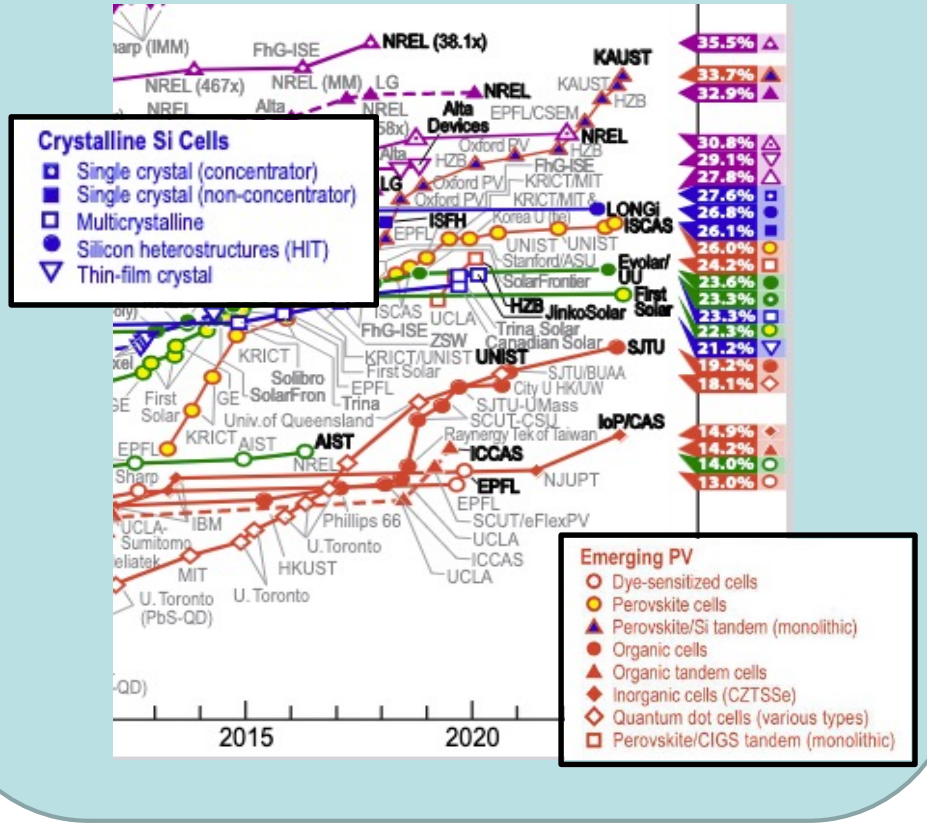
Good light harvester

Excellent photovoltaic performance

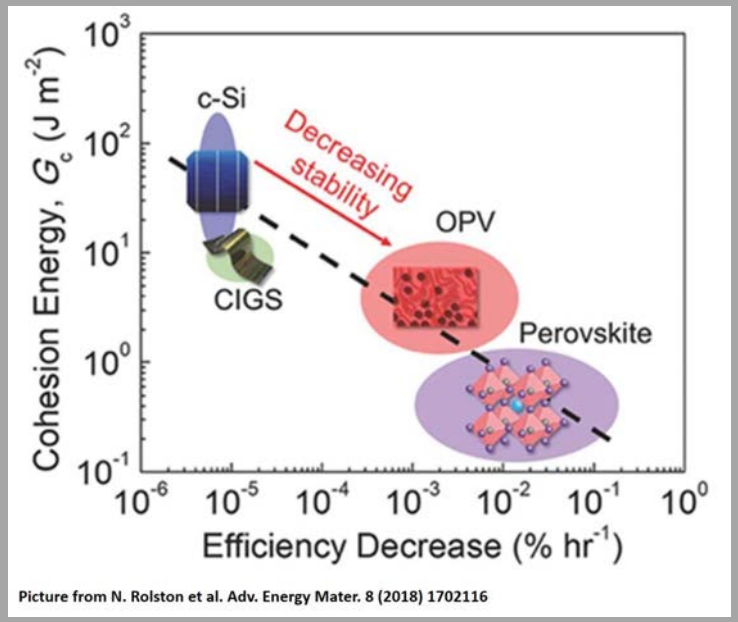
Concerns for stability

- Scientific & technical challenges addressed

The "bright" side

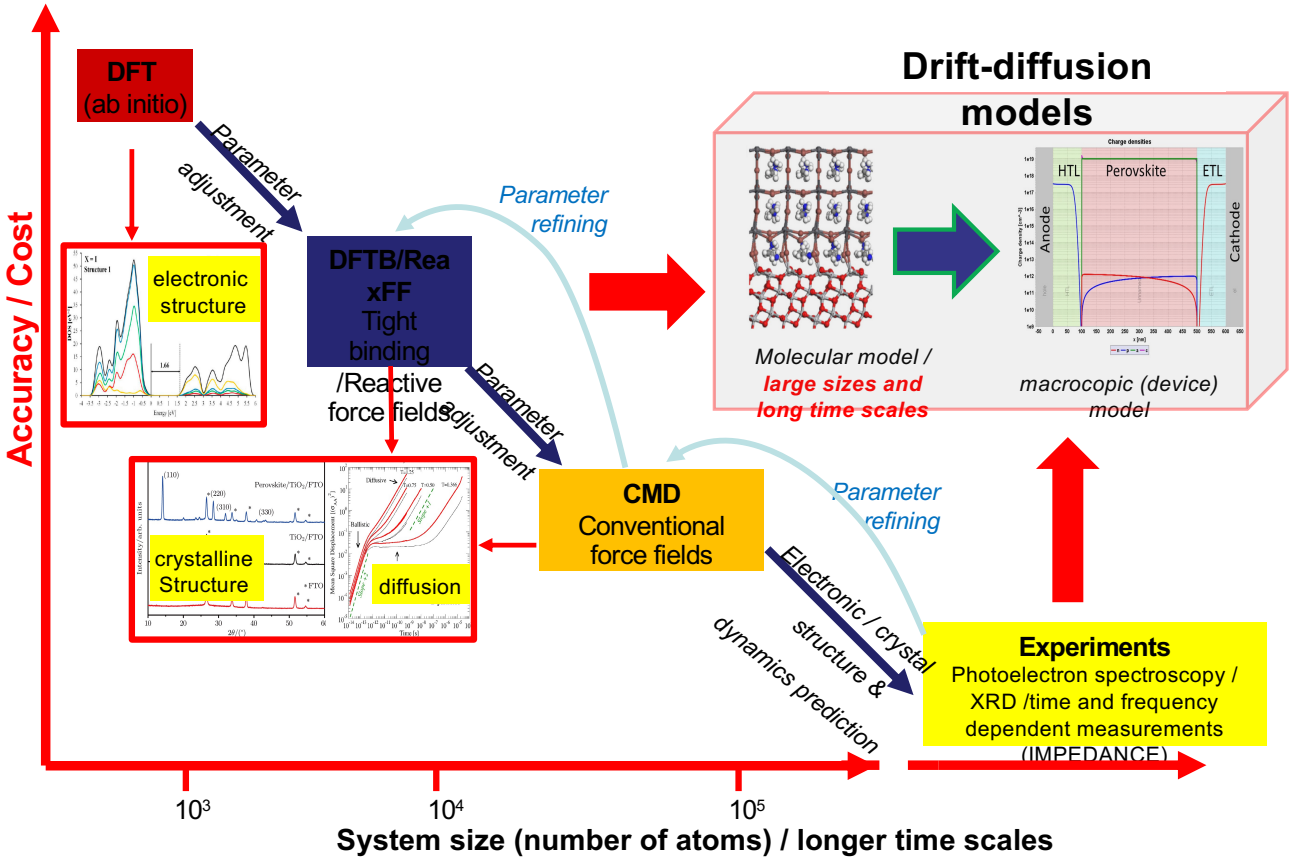


The "dark" side



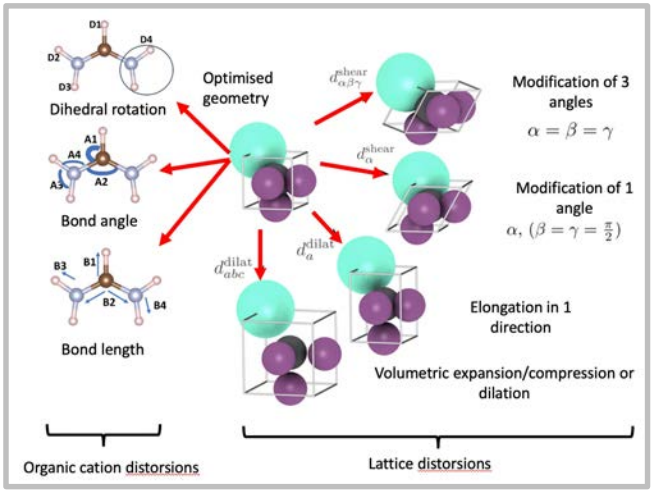
Picture from N. Rolston et al. Adv. Energy Mater. 8 (2018) 1702116

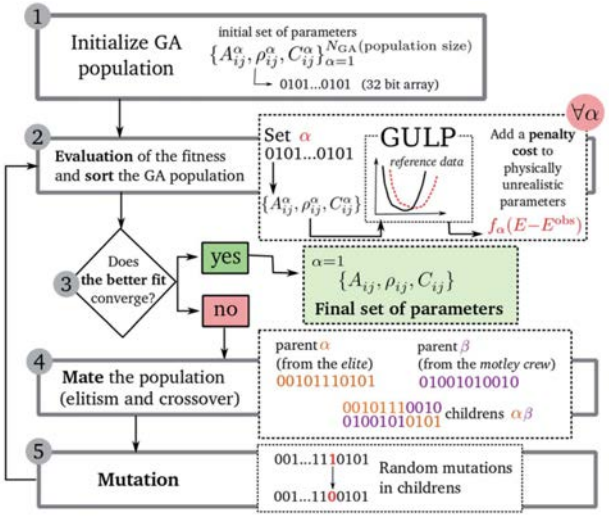
- Key outcomes, results and benefits

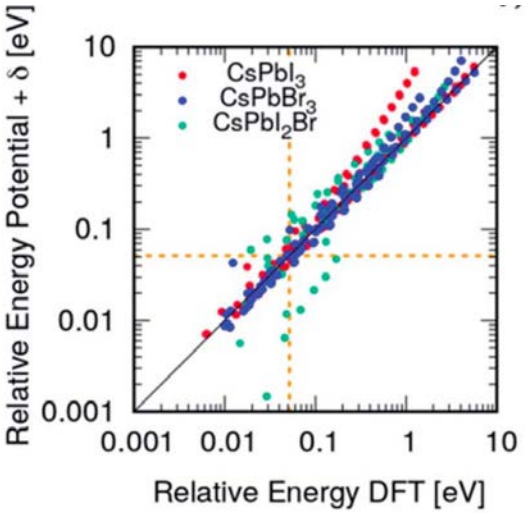


- Key outcomes, results and benefits

First principles calculations for a variey of configurations → Development of genetic algorithms for parameters fitting → Materials Properties prediction



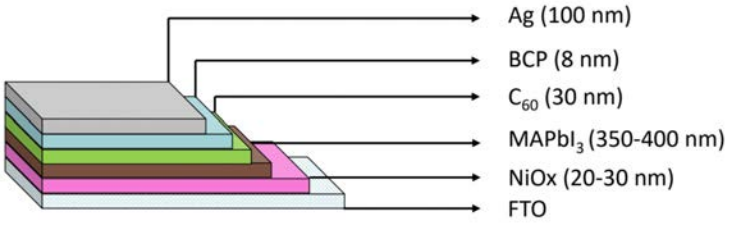


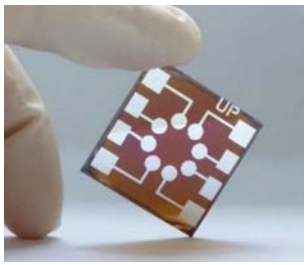


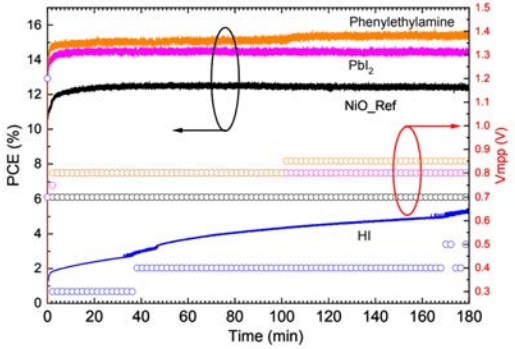
Balestra et al. 2020, *Efficient Modelling of ion Structure and Dynamics in Inorganic Metal Halide Perovskites*, Journal of Materials Chemistry A, (2020)

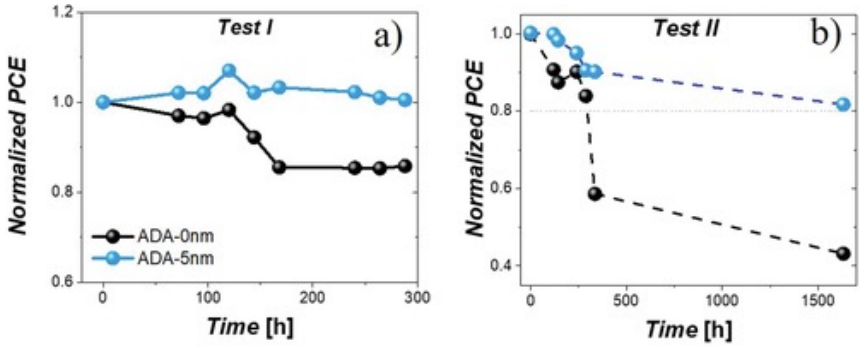
Seijas-Bellido et al. *Transferable Classical Force Field for Pure and Mixed Metal Halide Perovskites Parameterized from First-Principles*. Journal of Chemical Information and Modeling

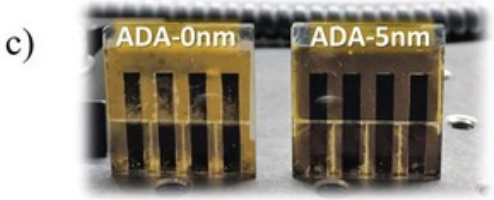
- Key outcomes, results and benefits





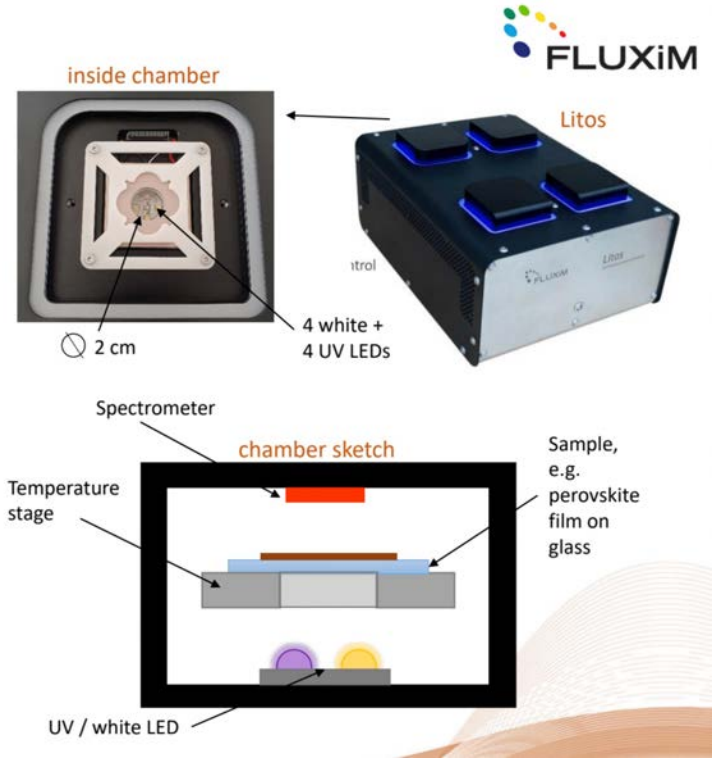


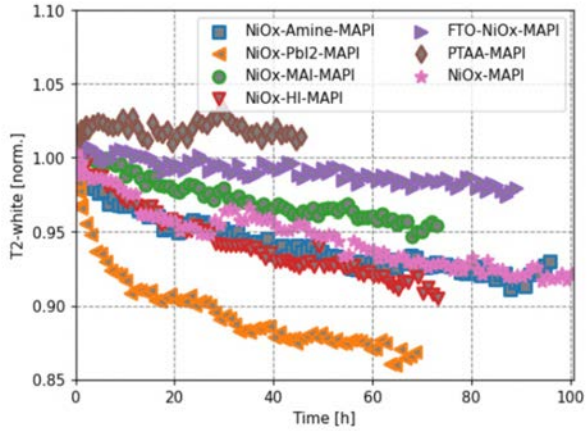


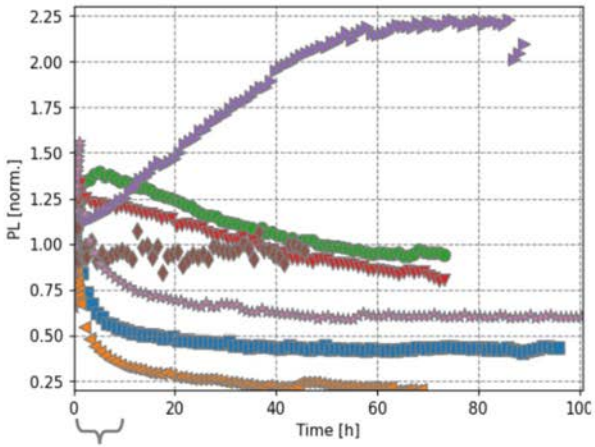


Obrero-Pérez et al. 2022, *Ultrathin Plasma Polymer Passivation of Perovskite Solar Cells for Improved Stability and Reproducibility*, Advanced Energy Materials, **2022**, 12, 32

- Key outcomes, results and benefits







Experiences gained in transnational set-up

- Productive cooperation between experimental and theoretical teams, despite differences in their approaches or perspectives.
- Productive cooperation between academic and industrial partners, despite differences in their interests and expectations
- Beneficial exchange of

  (1) students/postdocs,
  (2) experimental and theoretical protocols,
  (3) chemicals, test samples and devices

Critical factors and lessons learned for future successful transnational R&I projects

- The pandemic at the beginning of the project complicated and disturbed (not critically) the experimental work plan (not a general issue though)
- The signature of the Consortium Agreement turned out to be sort of traumatic: very different views between the administrative staff and the scientific staff. The collaboration within the colleagues in the consortium was, in spite of this, smooth, fruitful and friendly
- We experienced problems in finding and hiring postdocs due to the lack of suitable candidates