Machine-Learning-Assisted Design Guideline of Capping Layer for Improving Perovskite Solar Cells Stability

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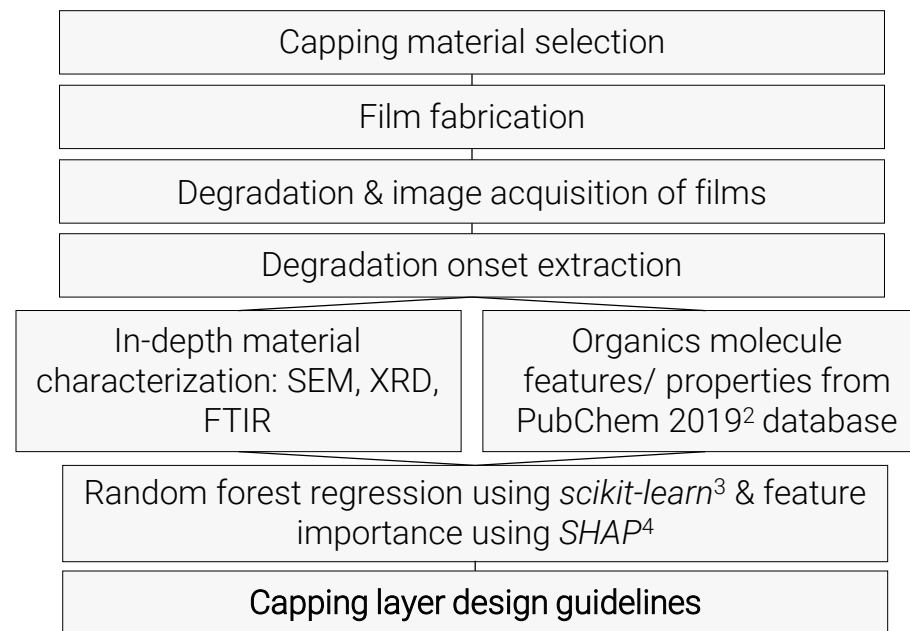[2]Brookhaven National Laboratory, Upton, NY 11973, USA
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Motivations

2D capping layer
3D MAPI
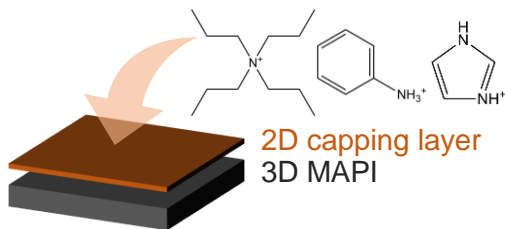
- 2D perovskite on top of perovskite absorber (capping layer) improves environmental stability.[1]
- Various organic *A*-site cations have been explored for this purpose.
- It is unclear how researchers can choose capping layer materials for optimum stability.
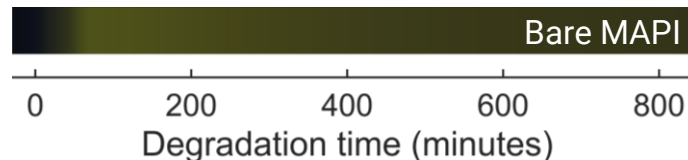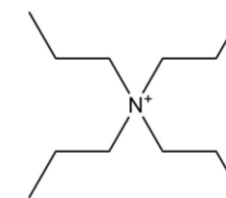
Experimental Method

Capping material selection

Film fabrication

Degradation & image acquisition of films

Degradation onset extraction

In-depth material characterization: SEM, XRD, FTIR

Organics molecule features/ properties from PubChem 2019[2] database

Random forest regression using *scikit-learn*[3] & feature importance using *SHAP*[4]

Capping layer design guidelines

Results and Discussion

Image Acquisition

With capping layer

TPABr $C_{12}H_{28}NBr$
TPAI $C_{12}H_{28}NI$
DAI $C_{12}H_{28}NI$
PTEAI $C_{12}H_{20}NI$

Without capping layer

Bare MAPI
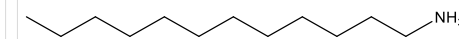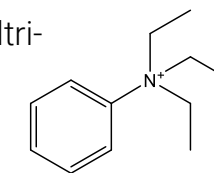
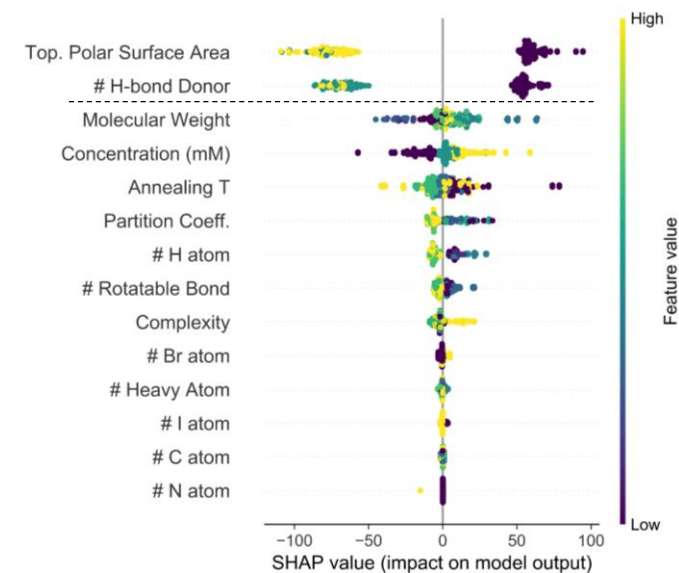TPA: tetrapropyl-ammonium

DA: dodecylammonium

PTEA: phenyltri-ethyl-ammonium

Molecular formulas are the same, but have different material properties.

Feature of Importance (FoI)

The stable capping layer materials have low number of Hydrogen-bond donor & small topological polar surface area.

References
1. Nature. 2019;567(7749):511-515. doi:10.1038/s41586-019-1036-3
2. Nucleic Acids Res. 2019;47(D1):D1102-D1109. doi:10.1093/nar/gky1033
3. http://arxiv.org/abs/1201.0490. Accessed September 20, 2019.
4. https://papers.nips.cc/paper/7062-a-unified-approach-to-interpreting-model-predictions. Accessed September 20, 2019.