Electronic Supplementary Material (ESI) for Energy Advances.


# Supporting Information

## Understanding Moisture Stability and Degradation Mechanisms in 2D Hybrid Perovskites: Insights from Ab Initio Molecular Dynamics Simulations

Eti Mahal,[†] Surya Sekhar Manna,[†] Sandeep Das, [†] and Biswarup Pathak[†]*

[†]Department of Chemistry, Indian Institute of Technology Indore, Indore 453552, India

*Email: biswarup@iiti.ac.in

## Contents

**Table S1:** Lattice parameters of all considered models.

| Phase | Cell Parameters | $PbI_2$ termination (Å) | I termination (Å) | Cation termination (Å) |
|---|---|---|---|---|
| **RP/$H_2O$** | *a* | 17.65 | 17.65 | 17.65 |
| | *b* | 17.14 | 17.14 | 17.14 |
| | *c* | 62.50 | 63.82 | 59.94 |
| **DJ/$H_2O$** | *a* | 18.32 | 18.32 | 18.32 |
| | *b* | 17.01 | 17.01 | 17.01 |
| | *c* | 51.00 | 53.74 | 48.62 |

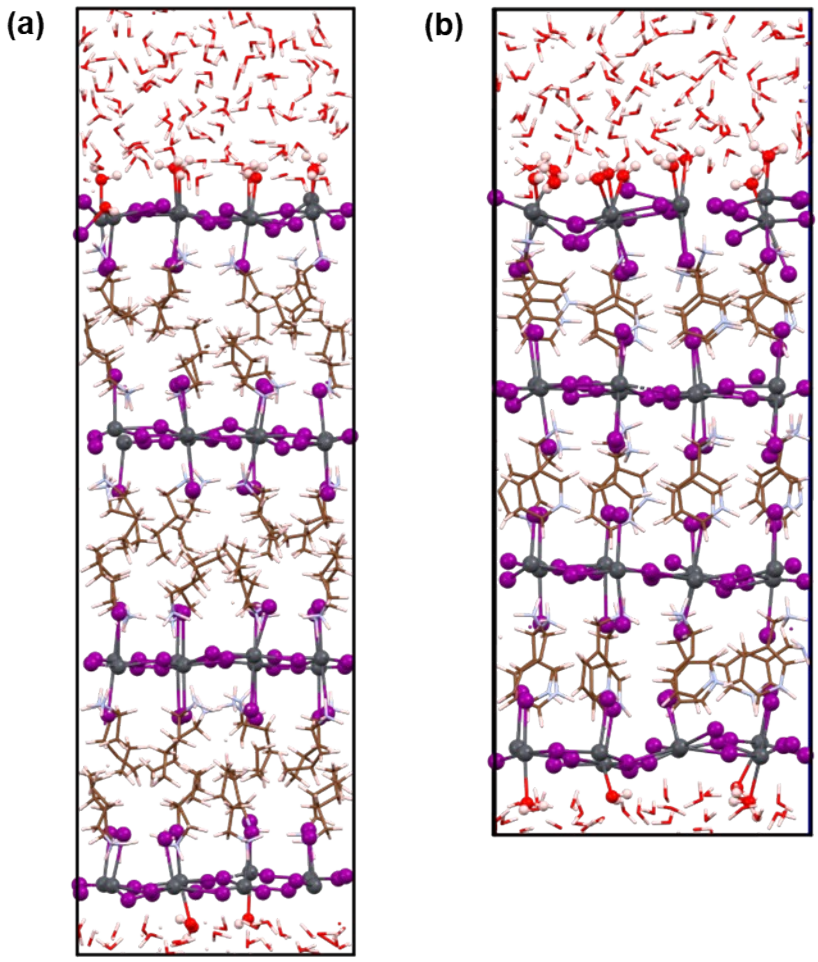


**Figure S1.** Post simulation geometries of $PbI_2$ terminated (a) RP/$H_2O$ interface and (b) DJ/$H_2O$ interface.

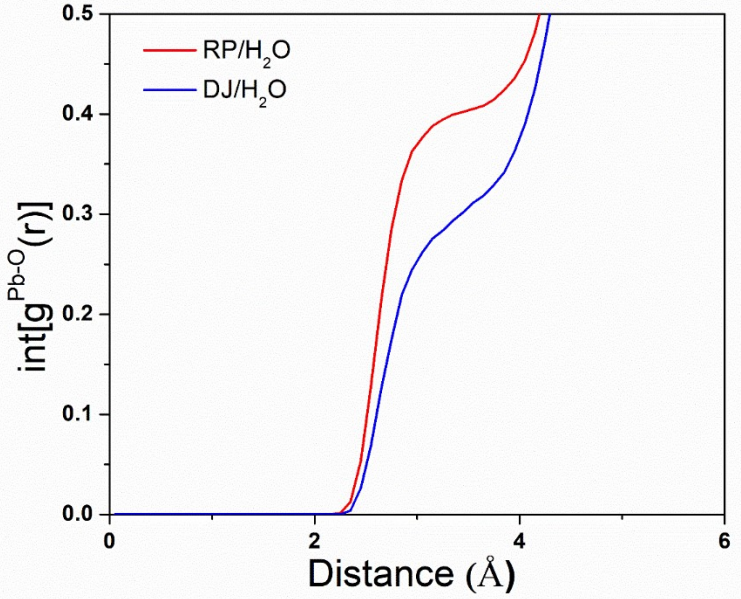


**Figure S2.** Integrated distribution plots of Pb−O radial pair distribution of $PbI_2$ terminated RP/$H_2O$ interface and DJ/$H_2O$ interface.

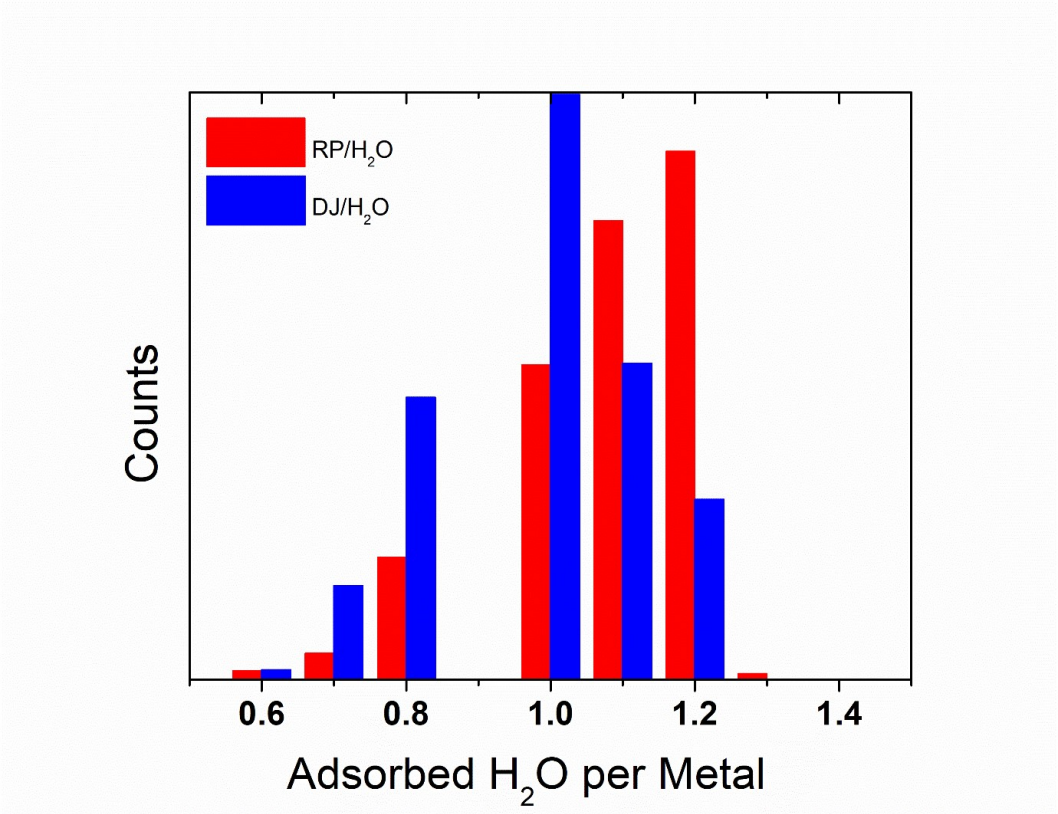


**Figure S3.** Histograms of the number of adsorbed waters per metal for the $PbI_2$ terminated water interfaces throughout the MD trajectories.

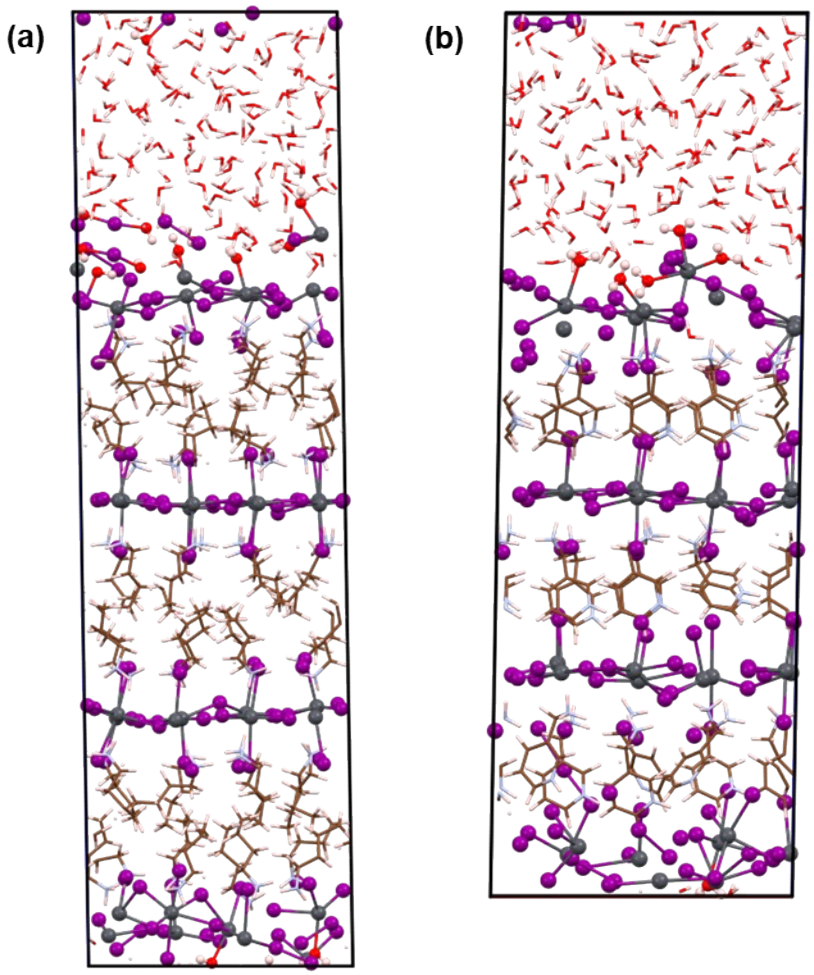


**Figure S4.** Post simulation geometries of I terminated (a) RP/$H_2O$ interface and (b) DJ/$H_2O$ interface.

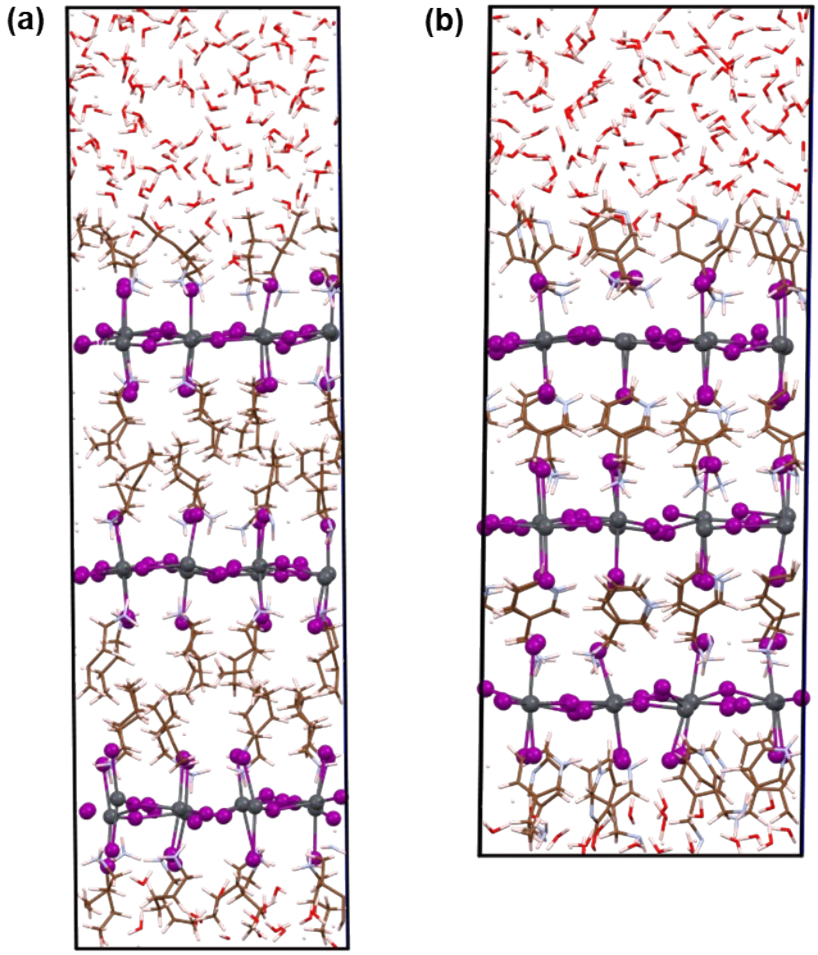


**Figure S5.** Post simulation geometries of cation terminated (a) RP/$H_2O$ interface and (b) DJ/$H_2O$ interface.