

Supporting Information

**Moderate intensity ligand works best: a theoretical study on  
passivation effects of pyridine-based molecules for perovskite solar  
cells**

Na Chen, Weiyi Zhang, Quan-Song Li\*

Key Laboratory of Cluster Science of Ministry of Education

Beijing Key Laboratory of Photoelectronic/Electrophotonic Conversion Materials

School of Chemistry and Chemical Engineering

Beijing Institute of Technology, 100081 Beijing, China

E-mail: [liquansong@bit.edu.cn](mailto:liquansong@bit.edu.cn)

## Supporting Information

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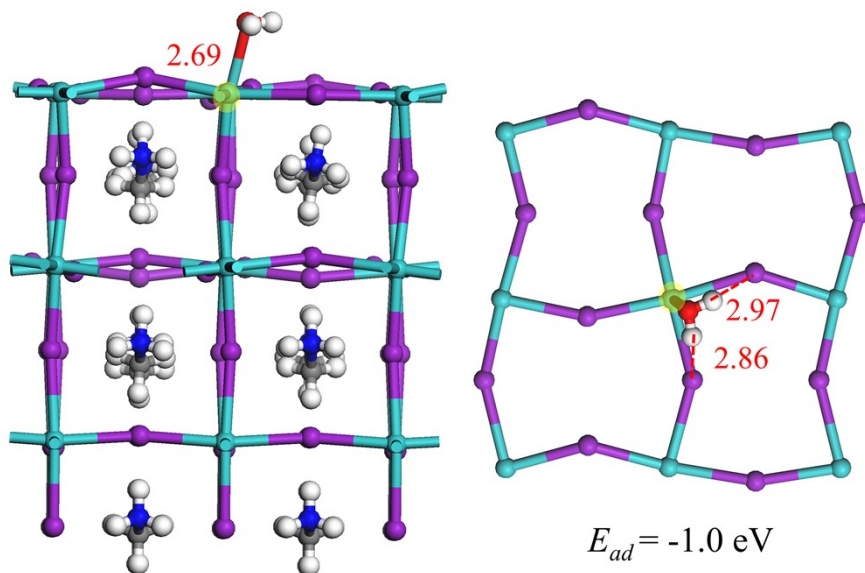


Figure S1. The adsorption configuration of  $H_2O@MAPbI_3$ .

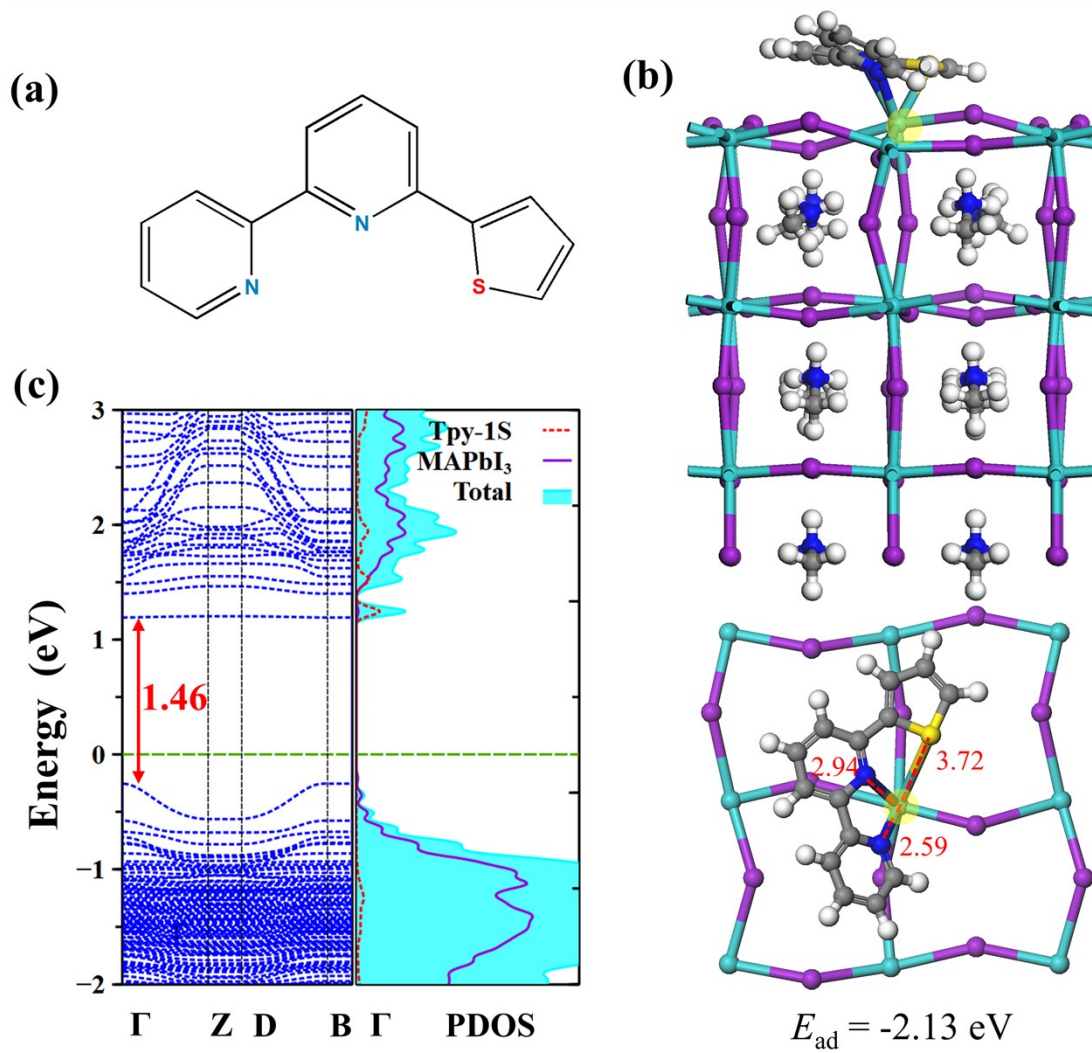


Figure S2. (a) Structure of Tpy-1S, (b) optimized adsorption configuration and (c) band structure and projected density of states (PDOS) for Tpy-1S@MAPbI<sub>3</sub>.

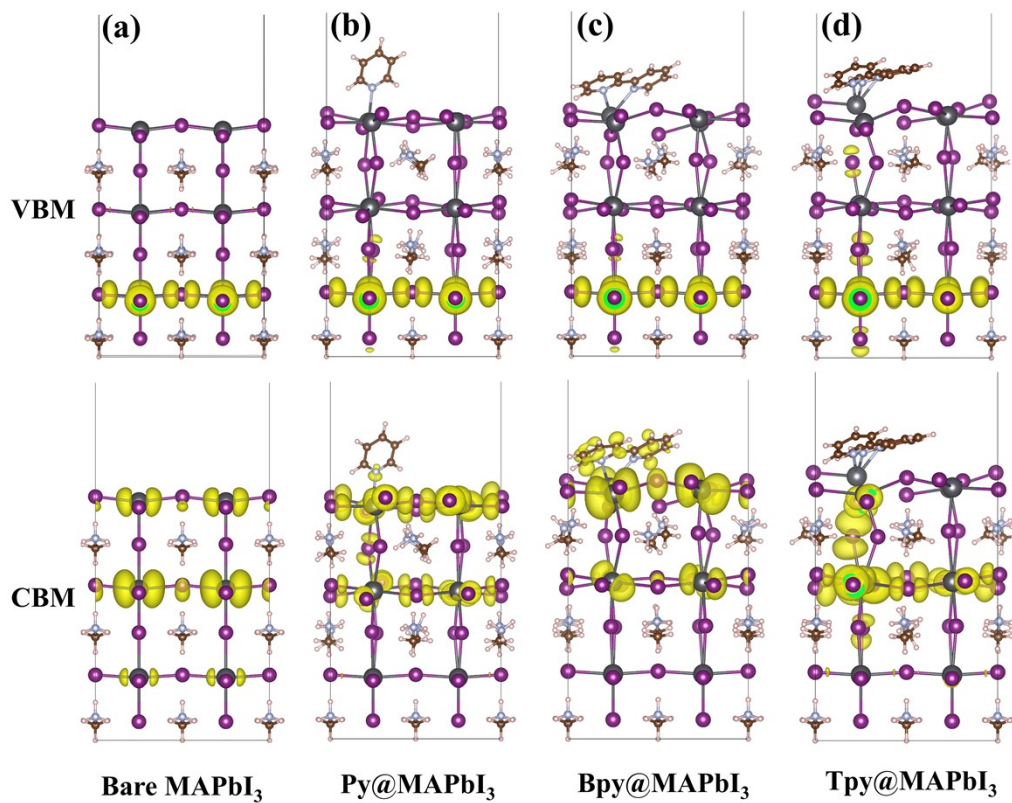


Figure S3. Charge densities of VBM and CBM for (a) bare MAPbI<sub>3</sub>, (b) Py@MAPbI<sub>3</sub>, (c) Bpy@MAPbI<sub>3</sub>, and (d) Tpy@MAPbI<sub>3</sub>, respectively. The isosurface level is 0.0008 e/Bohr<sup>3</sup>.

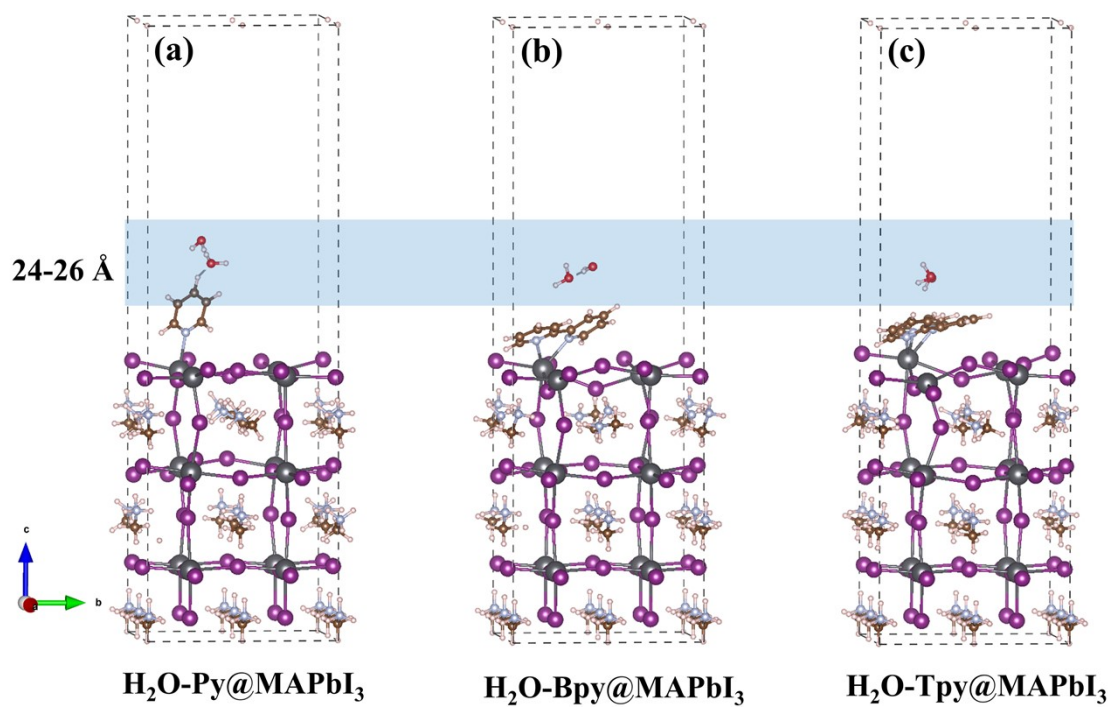


Figure S4. Initial AIMD configurations for  $\text{H}_2\text{O-PMs@MAPbI}_3$ .

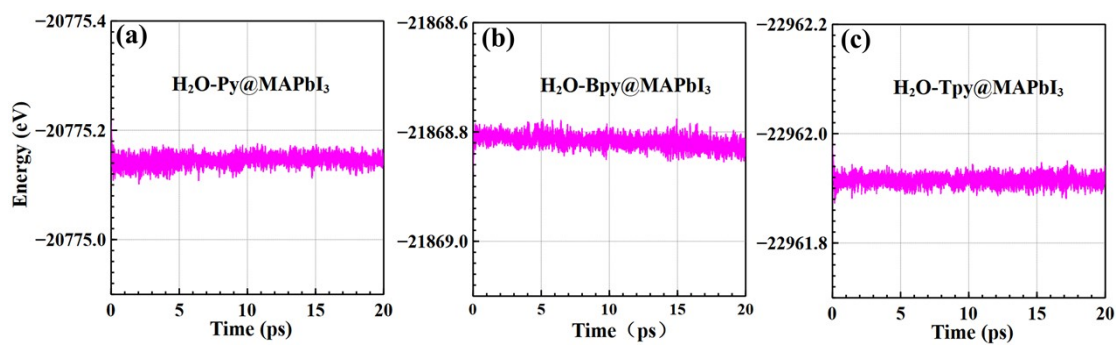


Figure S5. Time evolution of the energy fluctuations for H<sub>2</sub>O-PMs@MAPbI<sub>3</sub>.

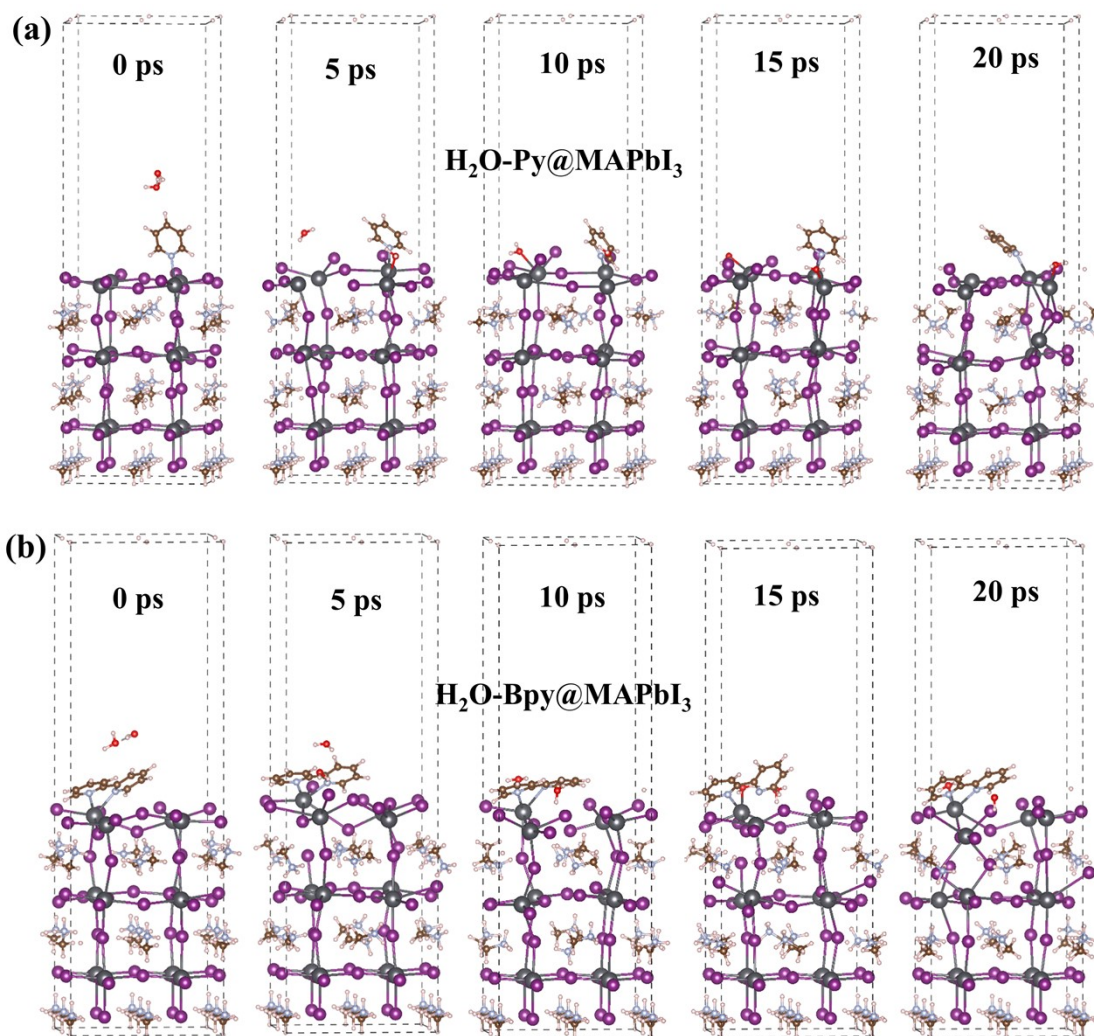


Figure S6. Snapshots of AIMD simulation at 0, 5, 10, 15, and 20 ps for (a)  $\text{H}_2\text{O-Py@MAPbI}_3$ , and (b)  $\text{H}_2\text{O-Bpy@MAPbI}_3$  systems at 300 K.