

Supporting information for:

Rational design of small molecule hole-transporting materials with linear π -bridge for highly efficient perovskite solar cells

Wenjing Zhu, Keyu Zhou, Yumeng Fo, Yi Li, Bin Guo, Xinyu Zhang,

Xin Zhou*

*College of Environment and Chemical Engineering, Dalian University, Dalian 116622,
Liaoning, China*

* Corresponding authors.

E-mail addresses: zhouxin@dlu.edu.cn.

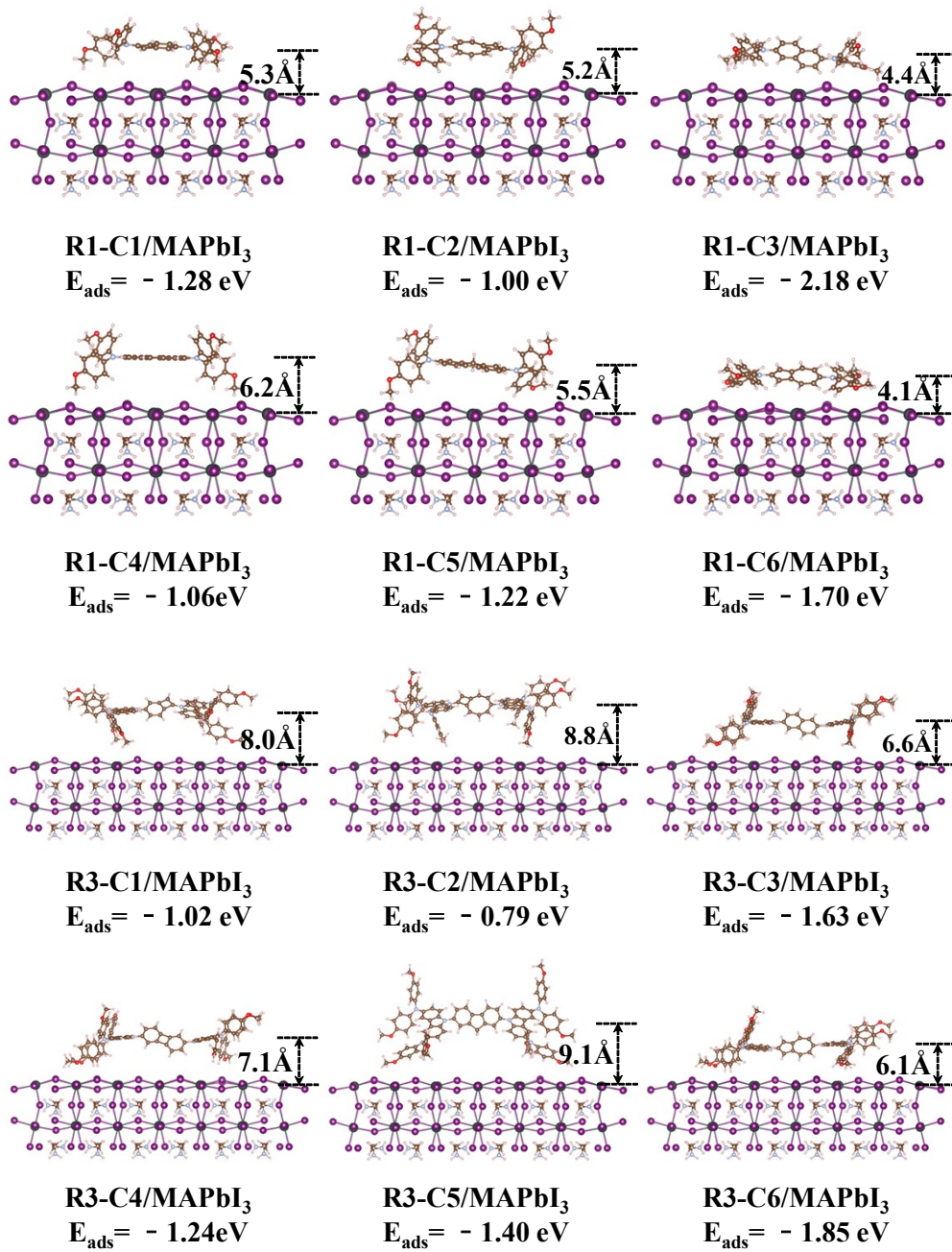


Fig. S1. The optimized structures and adsorption energy of R1-C_n and R3-C_n (n=1-6) absorbed on the PbI₂-terminated MAPbI₃(110) surface. The arrows indicate the distances between the MAPbI₃ surface and the centroid of HTM.