Supporting Information

Glue-like passivation of natural alkene lycopene for efficient and stable perovskite solar cells: insight from a theoretical perspective

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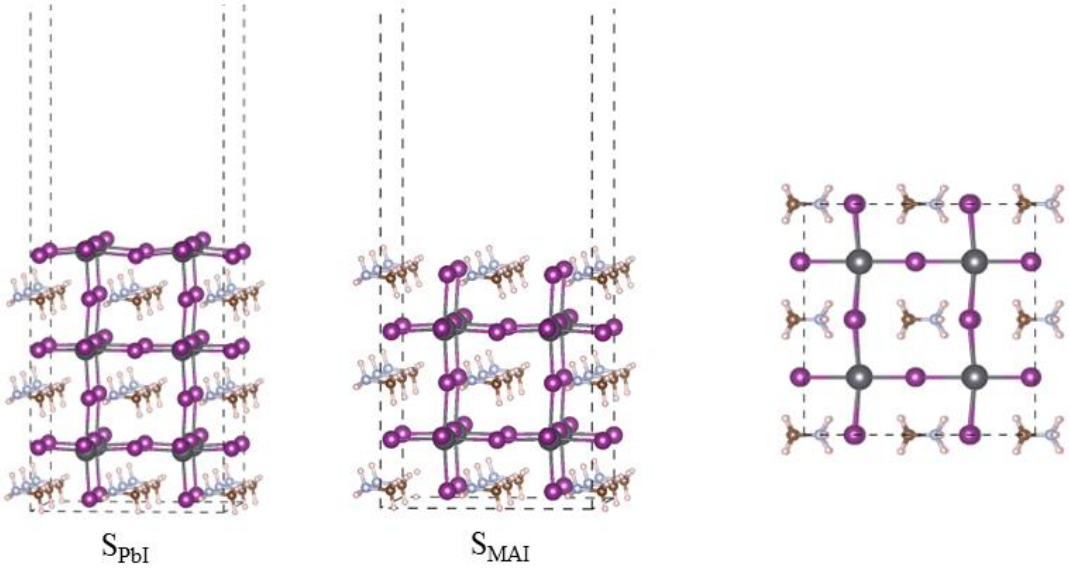

Figure S1. Side and top views of slab models of PbI_2-terminated ($S_{Pb–I}$) and MAI-terminated ($S_{MA–I}$) (001) surfaces of $MAPbI_3$.

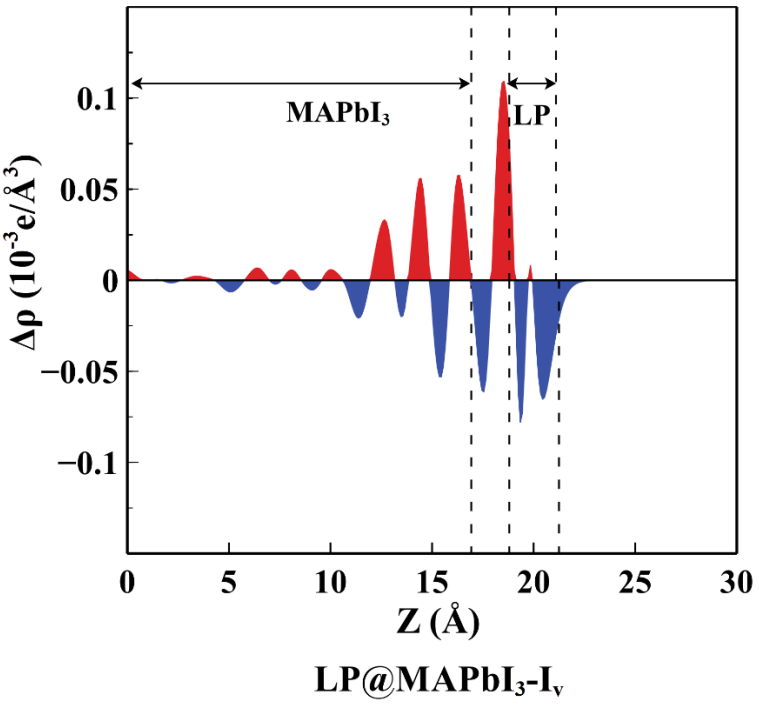

Figure S2. The planar-averaged charge density difference for LP@$MAPbI_3$-I_v along z direction. The positive value suggests the charge accumulation, and the negative value refers to the charge depletion.

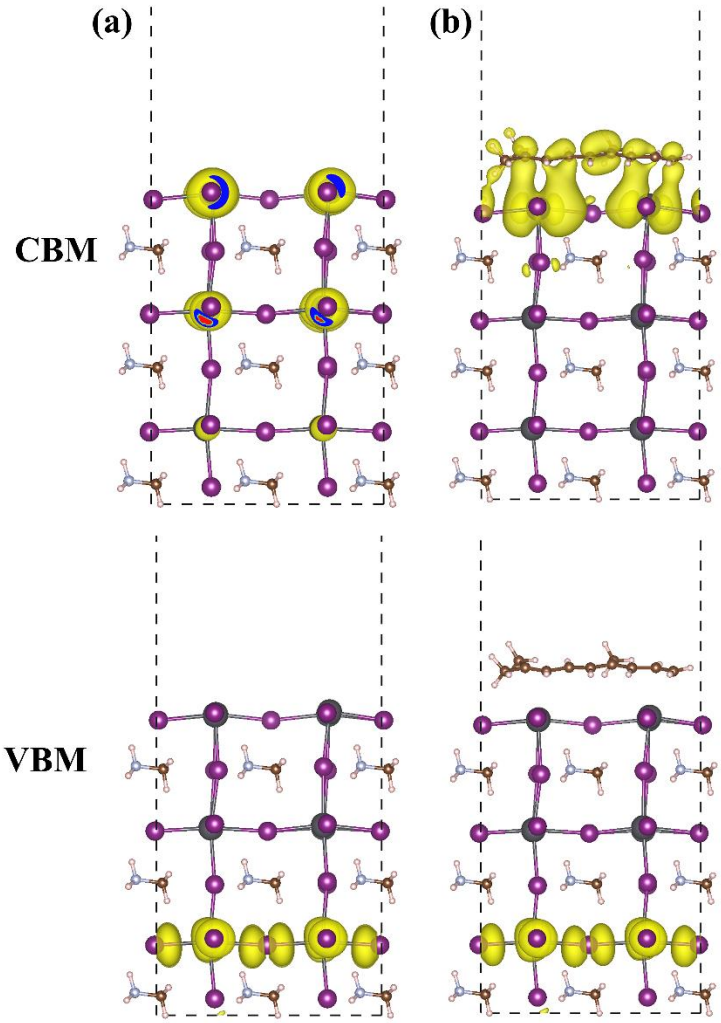

Figure S3. Charge densities of CBM and VBM for (a) $MAPbI_3$-I_v and (b) LP@$MAPbI_3$-I_v. The isosurface level is 0.0008 e/Bohr^3.

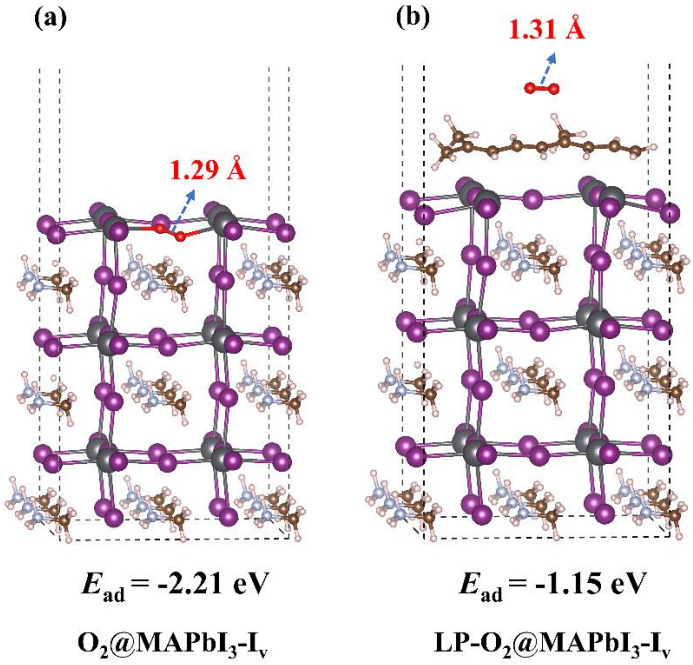

Figure S4. The side and top views of optimized configurations for (a) O_2@$MAPbI_3$-I_v and (b) LP-O_2@$MAPbI_3$-I_v.

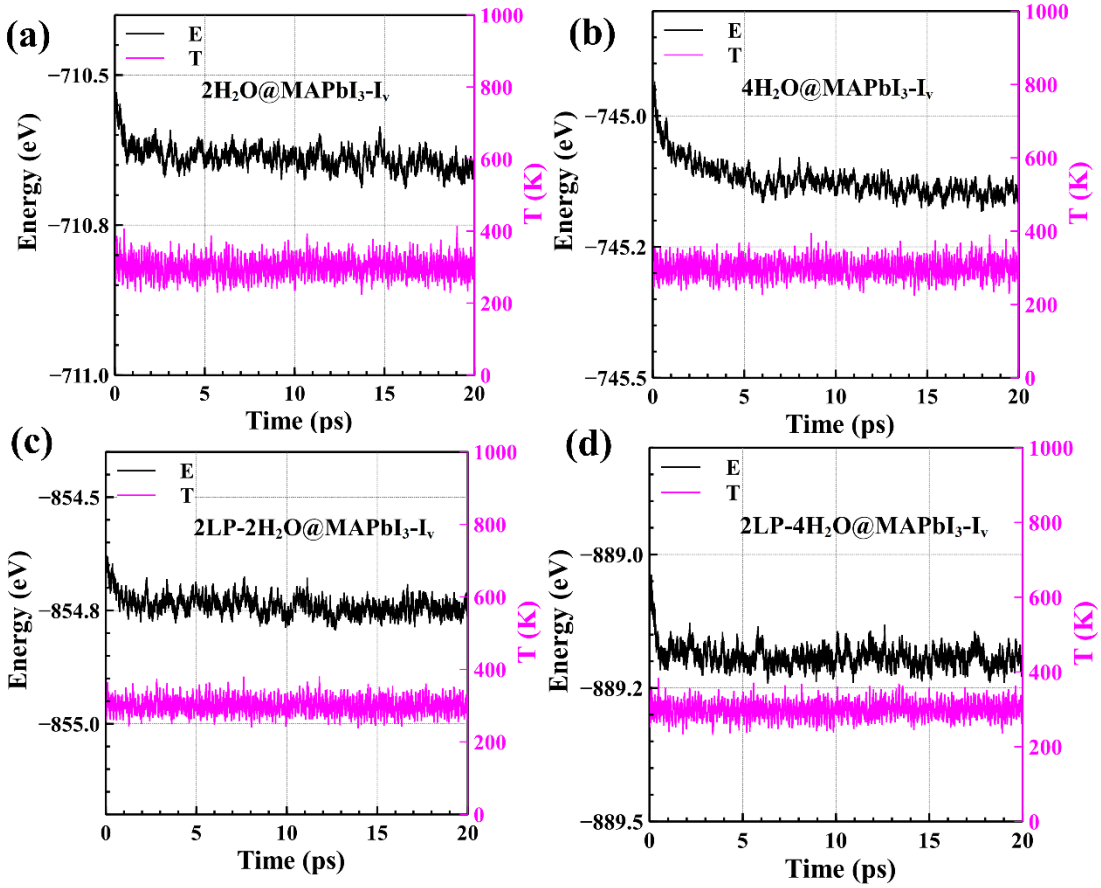

Figure S5. Energy evolution and temperature fluctuation for (a) $2H_2O@MAPbI_3$-I_v, (b) $4H_2O@MAPbI_3$-I_v, (c) 2LP-$2H_2O@MAPbI_3$-I_v and (d) 2LP-$4H_2O@MAPbI_3$-I_v.systems.

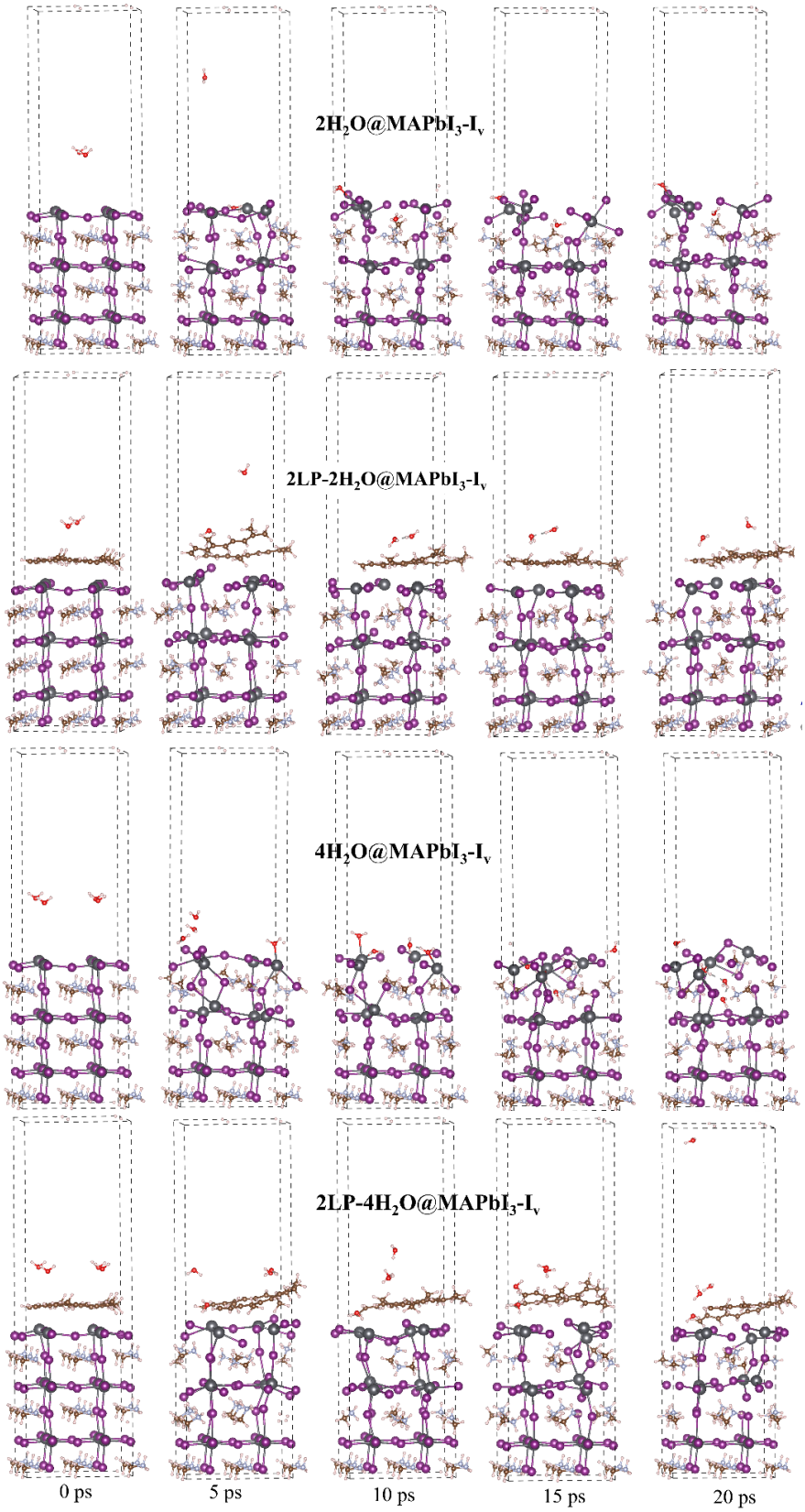

Figure S6. Snapshots of AIMD simulations at 0, 5, 10, 15, and 20 ps for $2H_2O$@$MAPbI_3$-I_v, 2LP-$2H_2O$@$MAPbI_3$-I_v, $4H_2O$@$MAPbI_3$-I_v, and 2LP-$4H_2O$@$MAPbI_3$-I_v.