

Electronic Supplementary Information

Cooperative multiple interactions of donor- π -acceptor dyes enhance the efficiency and stability of perovskite solar cells

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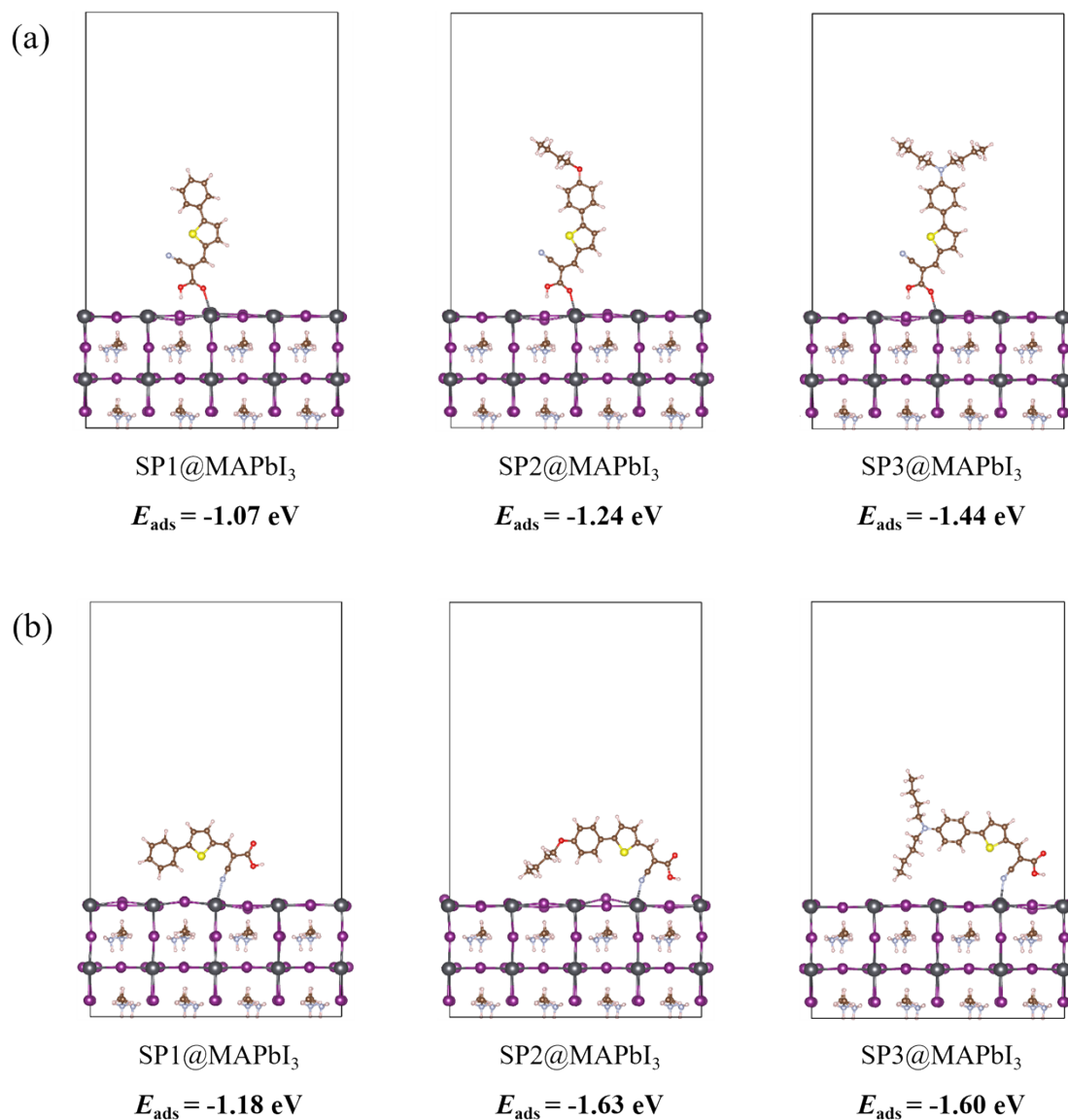


Fig. S1. Interfacial structures (a) by the vertical pattern and (b) by the lateral pattern of SP1@MAPbI₃, SP2@MAPbI₃, and SP3@MAPbI₃. The corresponding adsorption energy (E_{ads}) is labeled below. Colour code: red, O; blue, N; bright yellow, S; brown, C; white, H; purple, I; and leaden, Pb.

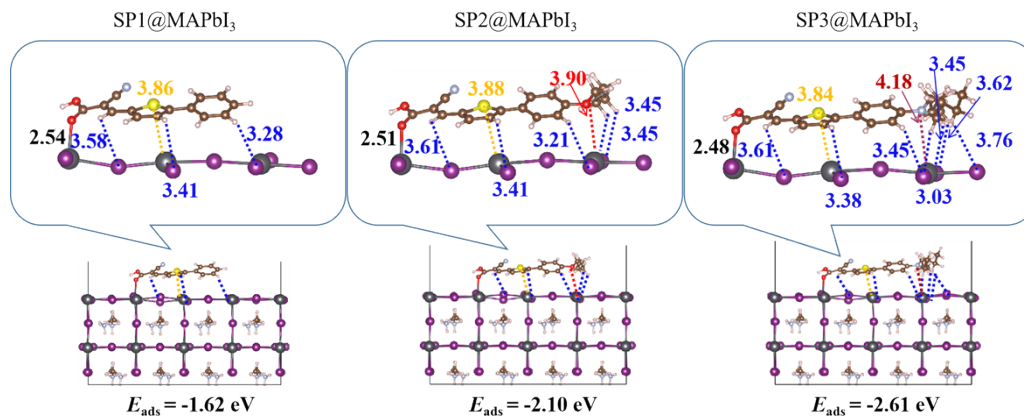


Fig. S2. Interfacial structures of SP1@MAPbI₃, SP2@MAPbI₃, and SP3@MAPbI₃. The I-H, S-Pb, N-Pb, and O_d-Pb bonds are marked in blue, yellow, dark red, and red, respectively. Colour code: red, O; blue, N; bright yellow, S; brown, C; white, H; purple, I; and leaden, Pb.

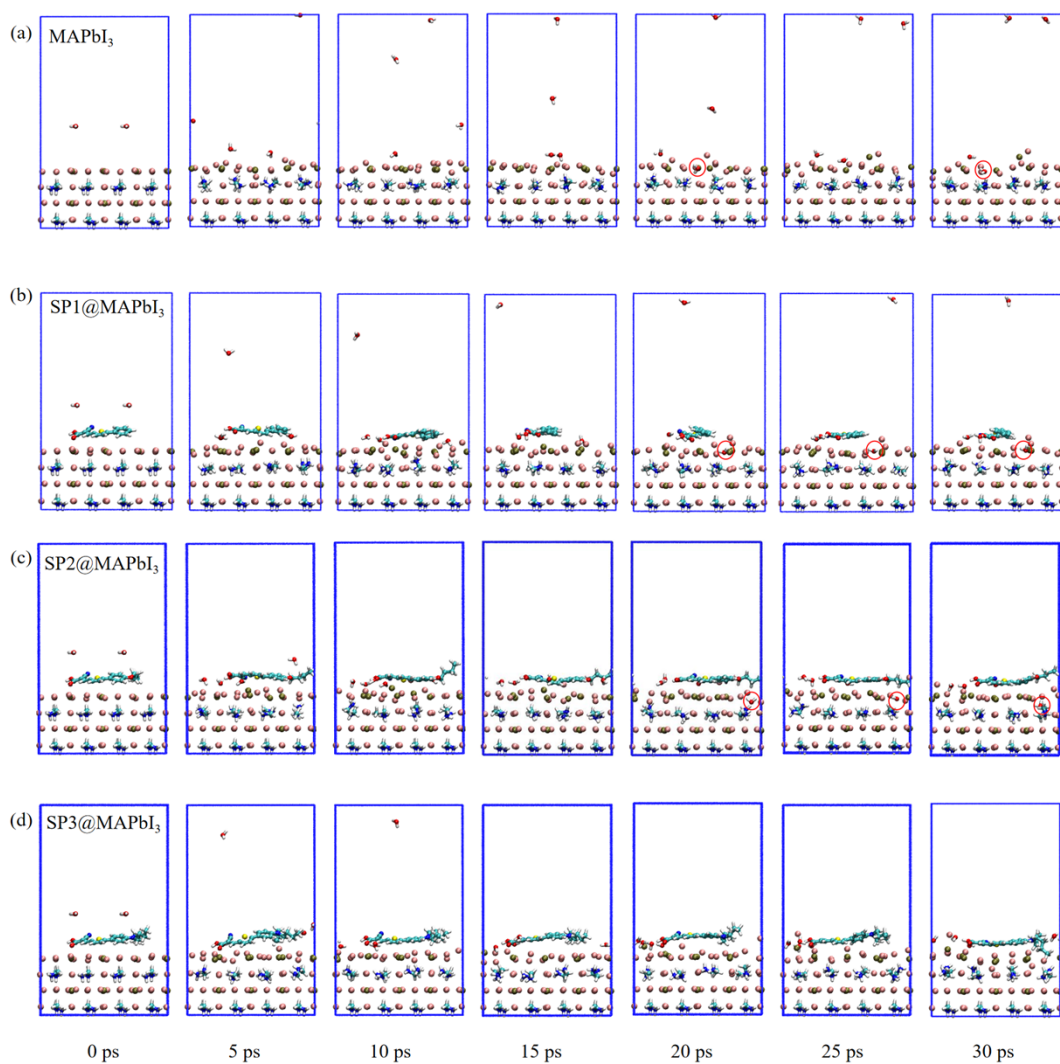


Fig. S3. Molecular dynamics of the water interaction with (a) pristine MAPbI₃, (b) SP1@MAPbI₃, (c) SP2@MAPbI₃, and (d) SP3@MAPbI₃, respectively. Snapshots at 0 ps, 5 ps, 10 ps, 15 ps, 20 ps, 25 ps, and 30 ps are depicted. Water entering the perovskite is highlighted with a red circle. Colour code: red, O; blue, N; bright yellow, S; cyan, C; white, H; pink, I; and dark gold, Pb.

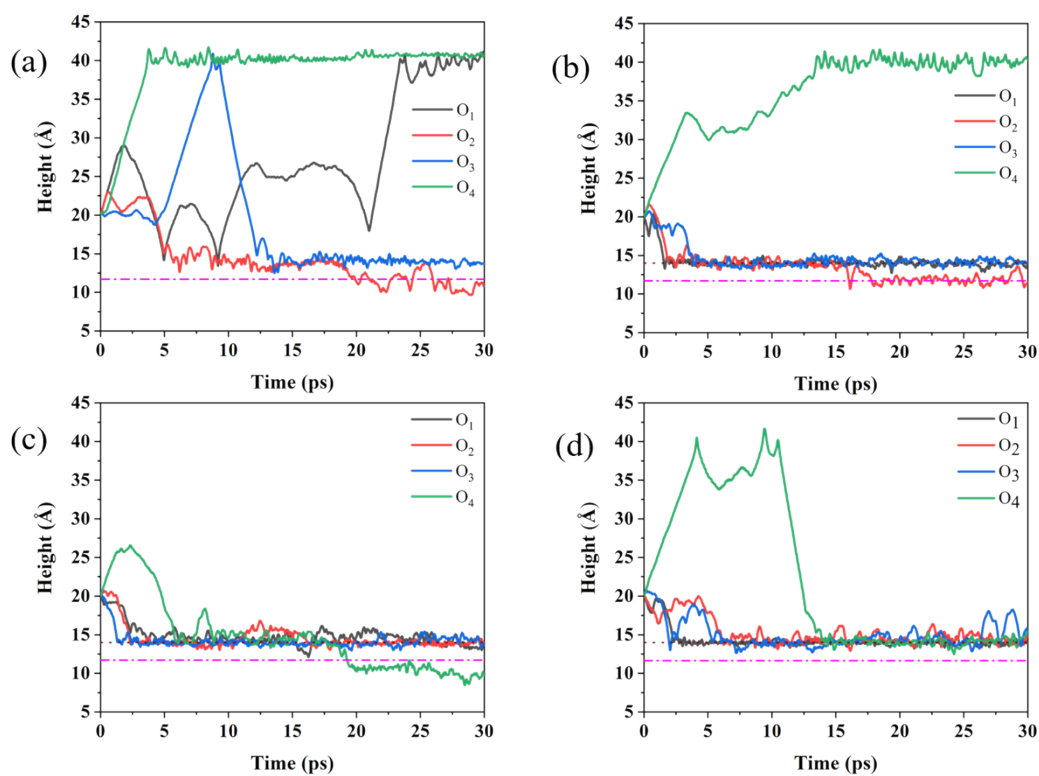


Fig. S4. Evolution of the height of the O atoms in water molecules for (a) MAPbI₃/H₂O, (b) SP1@MAPbI₃/H₂O, (c) SP2@MAPbI₃/H₂O, and (d) SP3@MAPbI₃/H₂O systems.