

Supporting information for

**Weak interactions in mixed symmetric and asymmetric self-assembled monolayers
for perovskite solar cells: a classical molecular dynamic view**

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This file includes: S1-S8

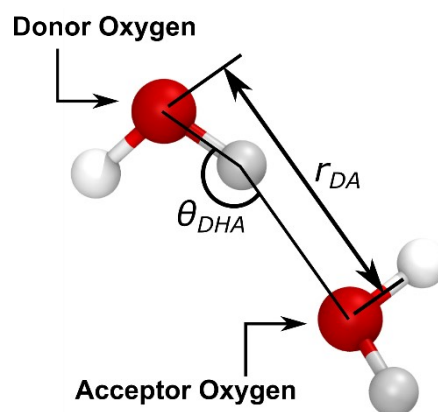


Fig. S1. The schematic diagram of hydrogen bond

π -Stacking Configuration

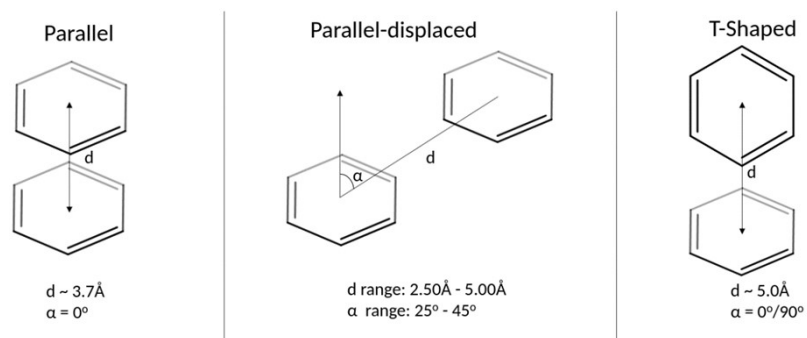


Fig. S2. The π - π interaction used in our analysis

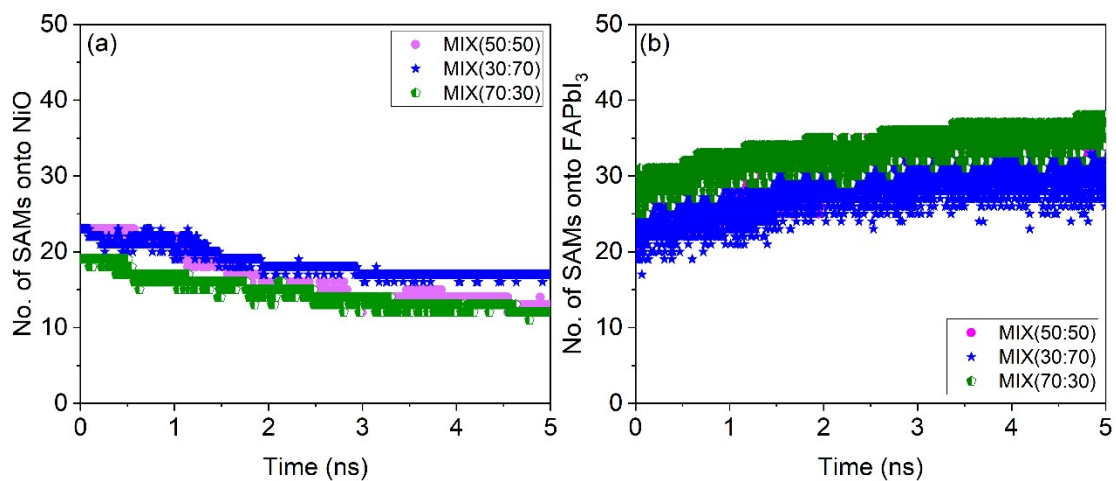


Fig. S3. The number of SAMs assigned to NiO and FAPbI₃ with different mix ratio

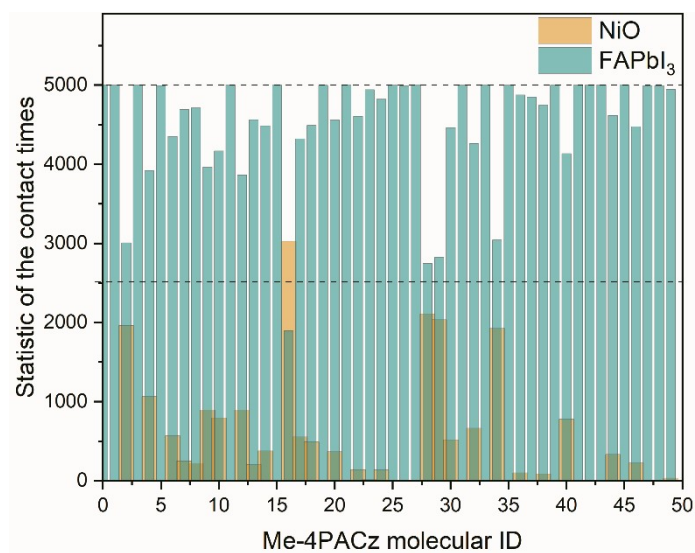


Fig. S4. The statistic of the contact times between Me-4PACz and NiO, FAPbI₃

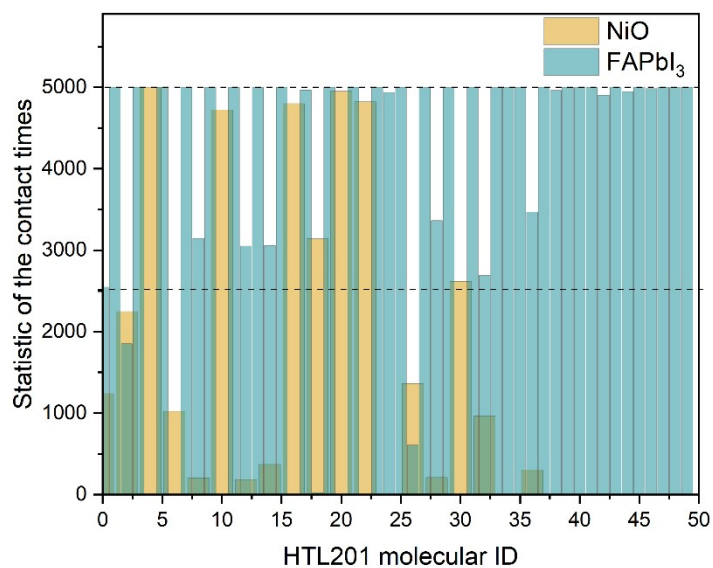


Fig. S5. The statistic of the contact times between HTL201 and NiO, FAPbI₃.

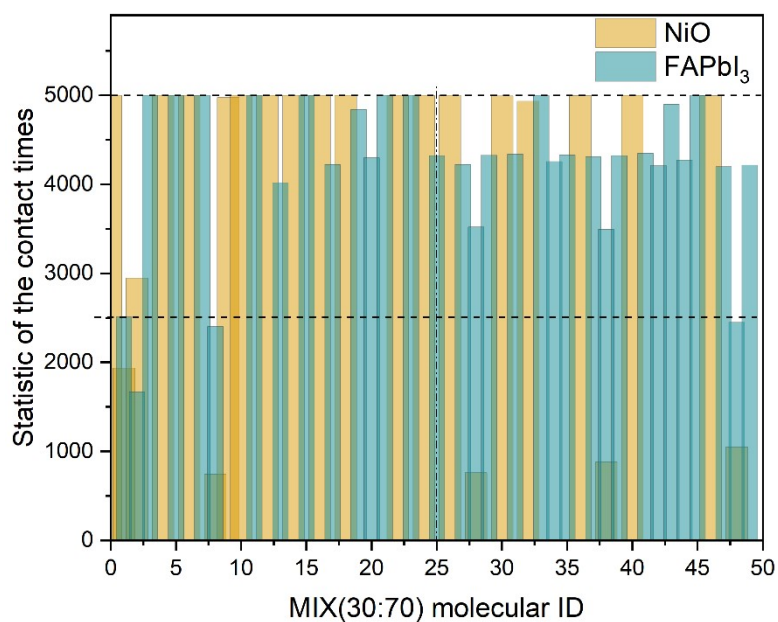


Fig. S6. The statistic of the contact times between MIX (30:70) and NiO, FAPbI₃.

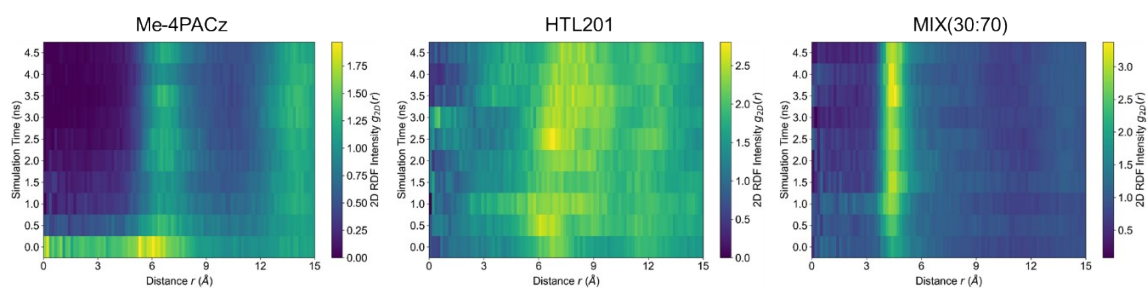


Fig. S7. RDF of the p-p atom pair during the 300 K 5ns production runs

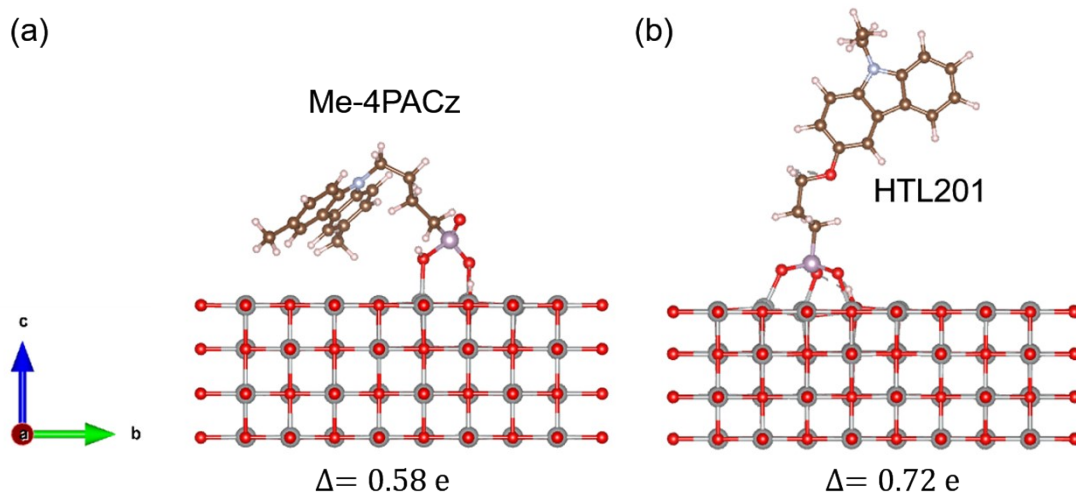


Fig. S8 Relaxed geometry of the Me-4PACz (a) and (HTL201) on NiO, the bade charge transfer is calculated.