Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Theoretical investigations on crystal crosslinking in perovskite solar cells

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Electronic Supplementary Information

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Table S1 Change in Hirshfeld charge in the adsorbate (the crosslinking agent) and adsorbent (the halide perovskite substrate) upon molecular adsorption on the perovskite substrate

	7	**8**	**9**
Crosslinking Agent	-0.39	-0.54	-0.64
Perovskite Substrate	0.39	0.54	0.64

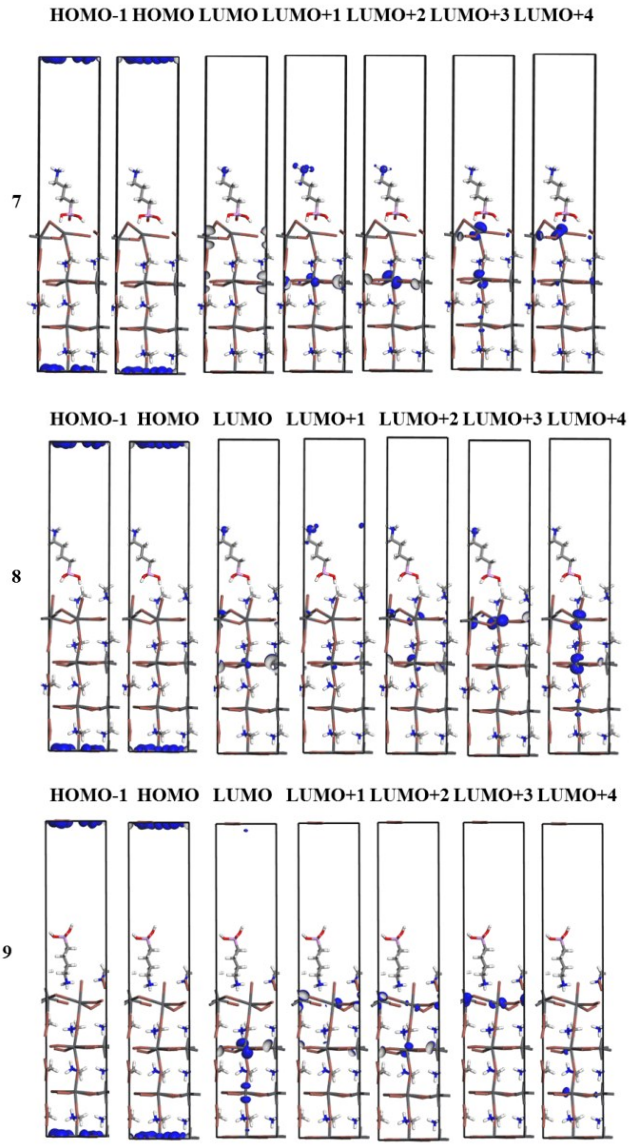

Figure S1 HOMO-1, HOMO, LUMO, LUMO+1, LUMO+2, LUMO+3 and LUMO+4 orbital distribution of **7-9**

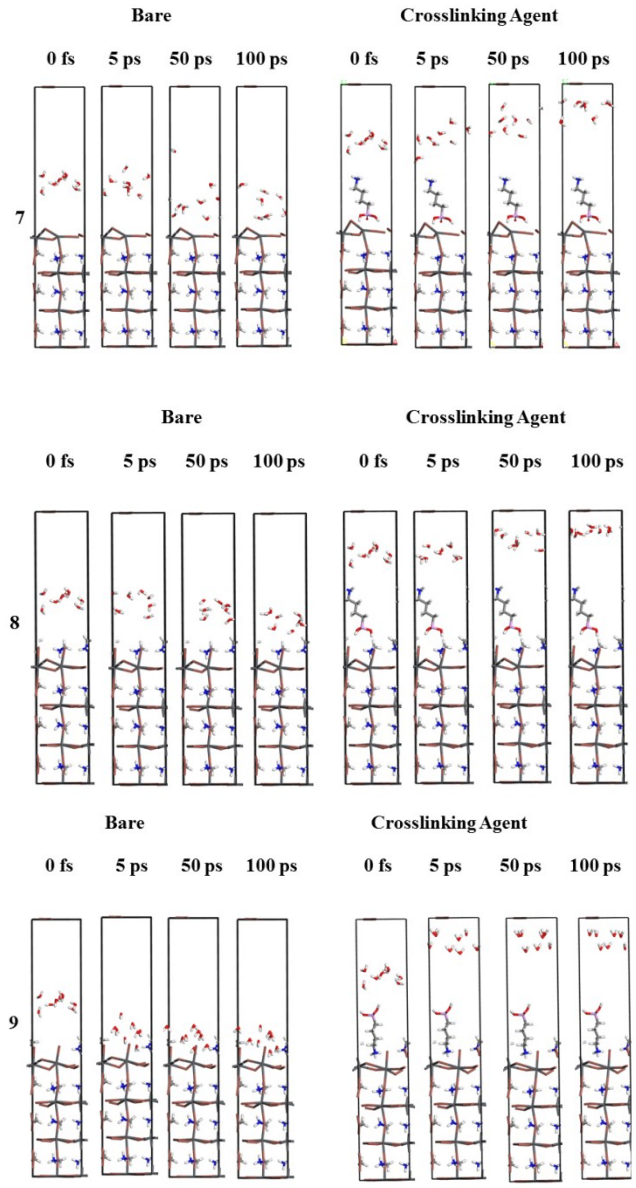

Figure S2 Molecular dynamics of the water interaction with the bare perovskite surface (left) and the perovskite surface capped by the crosslinking agents **7-9** (right). Snapshots at 0 fs, 4 ps, 40 ps and 100 ps are depicted in each case. Water molecules tend to approach the bare perovskite surface while they are expelled from the capped perovskite surface during the simulation time.

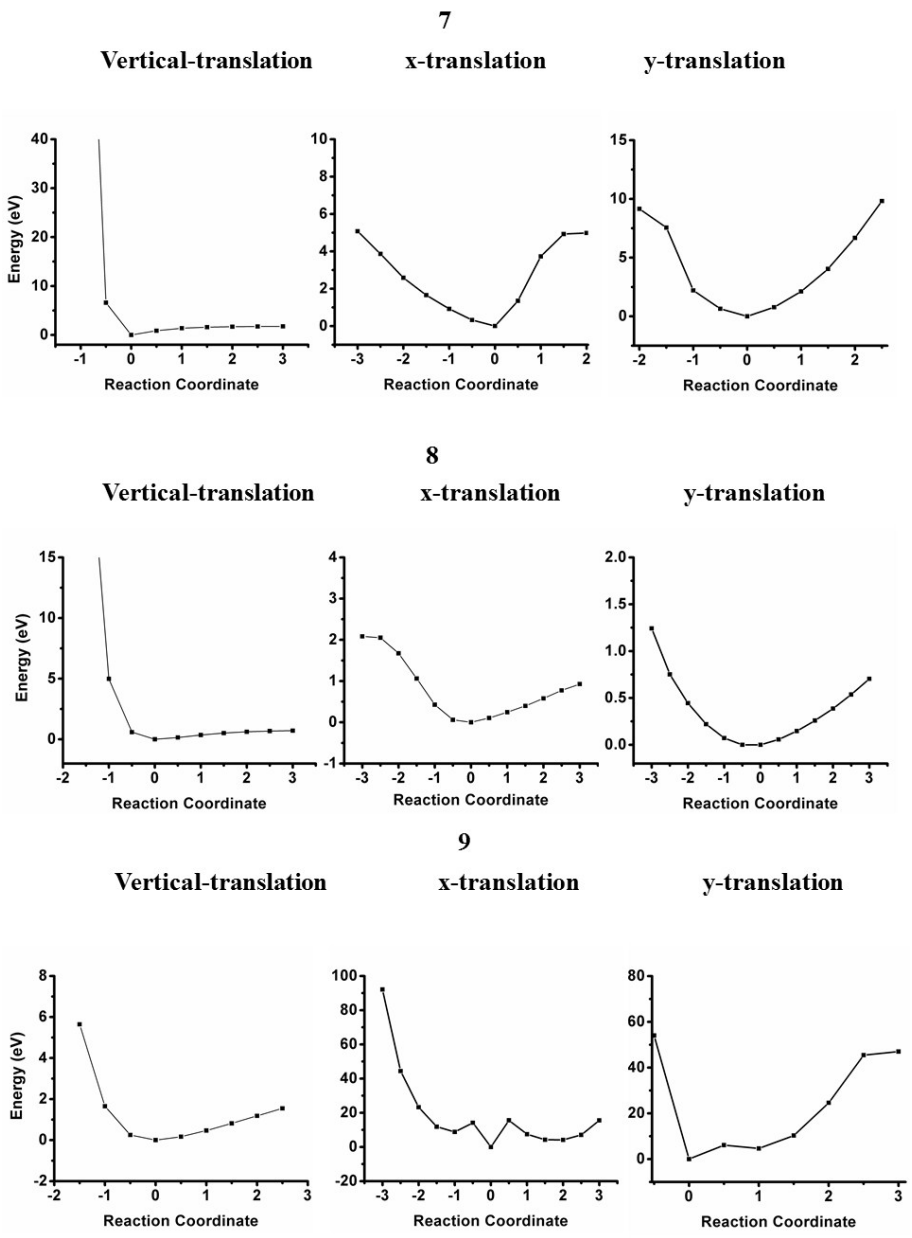

Figure S3 Relative energies along three reaction coordinates (vertical translation along z-axis, x-translation and y-translation of the adsorbate at the perovskite surface) for **7**-**9**. The optimized stable position is set to 0.

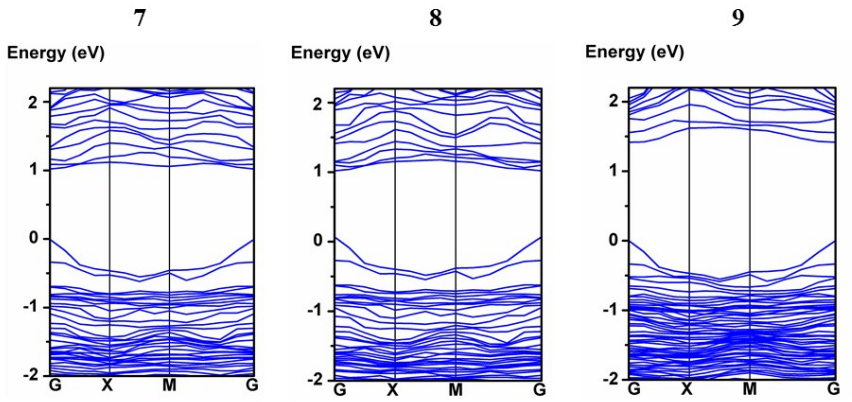

Figure S4 The band structures of **7-9** along lines connecting high symmetry points G (0, 0, 0), X (0, 0.5, 0), M (0.5, 0.5, 0) and G (0, 0, 0). The maximum energy of valence band is set to 0.

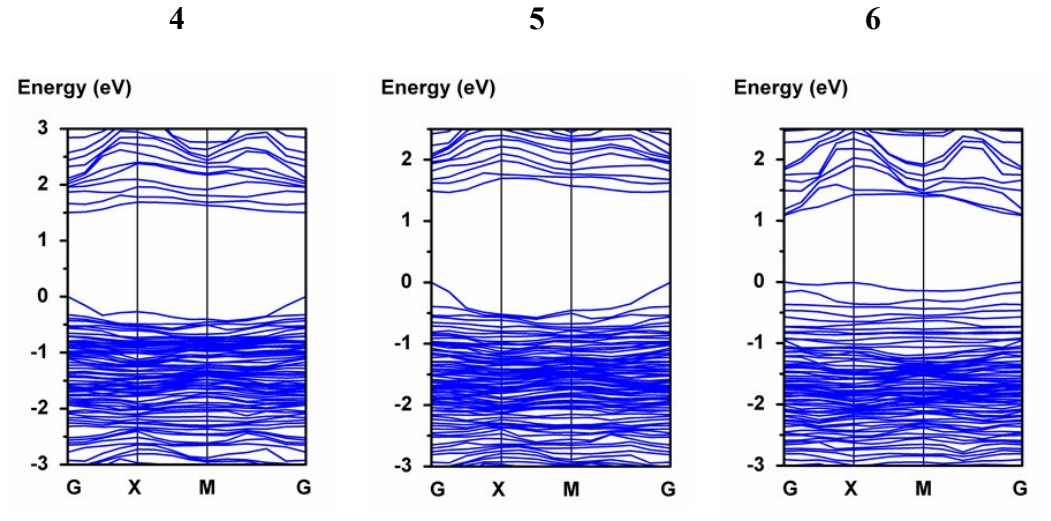

Figure S5 Band structures of **4-6**. The band gaps are 1.51 eV in **4** (1.51 eV from reference [1]), 1.47 eV (1.36 eV from reference [2]) in 5, and 1.09 eV in **6**. The Experimental values are 1.55 – 1.70 eV.[2–4]

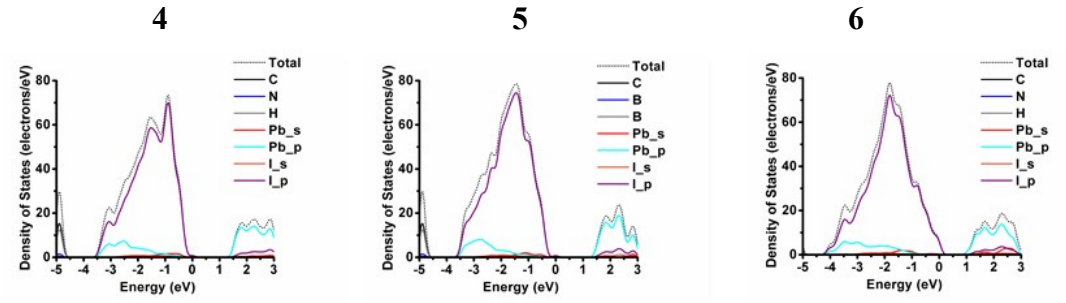

Figure S6 PDOS of **4-6** from -5 eV to 3 eV. In PDOS, the valence band is mainly contributed by the p orbital of I atoms and slightly by the s orbital of Pb atoms, while the conduction band is mainly contributed by the p orbital of Pb atoms and slightly by the s orbital of I atoms. These are consistent with the literature.[1,5–7]

References

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