Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information for On the Adsorption Mechanism of Caffeine on $MAPbI_3$ Perovskite Surfaces: A Combined UMC–DFT Study

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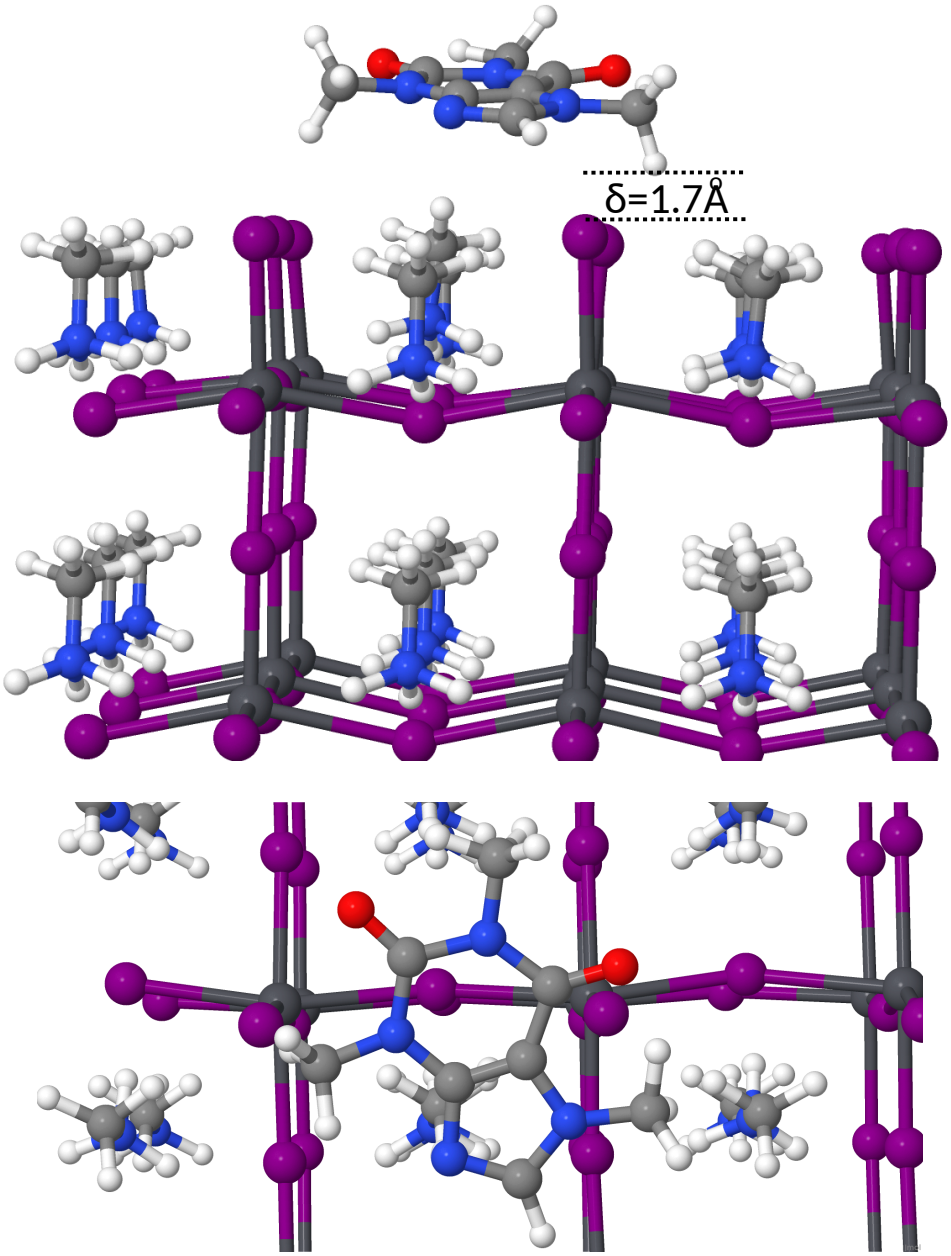

FIG. S1. DFT ground state configuration for the Methyl-ammonium covered PbI_3 perovskite. The caffeine/$MAPbI_3$ adsorption energy is $E_0 = -1.14$ eV. A Mulliken charge of $-0.334e$ is transferred from caffeine to $MAPbI_3$ perovskite. δ denotes the distance between the caffeine molecule and the perovskite surface.

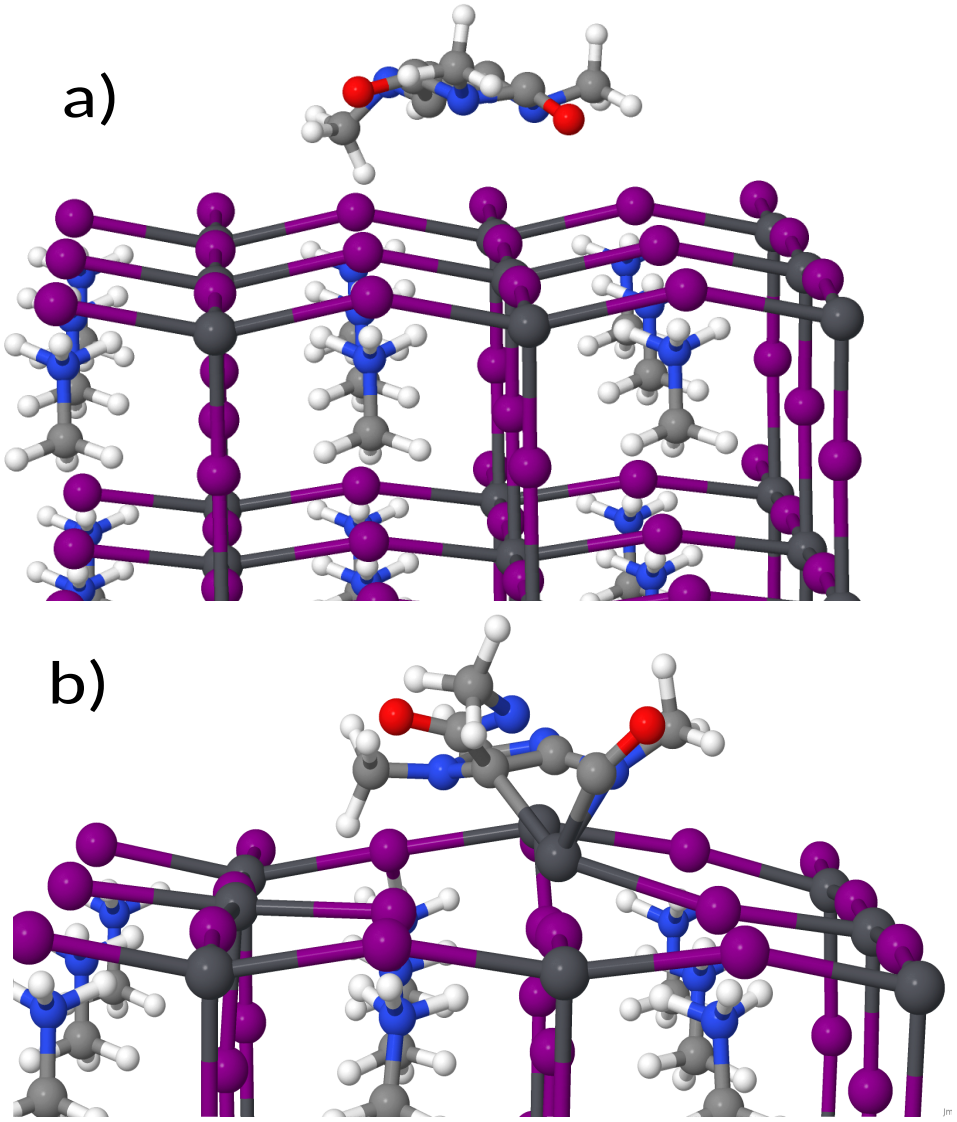

FIG. S2. Pb covered PbI_3 perovskite interaction with a caffeine molecule: a) input structure and b) obtained DFT ground state configuration.

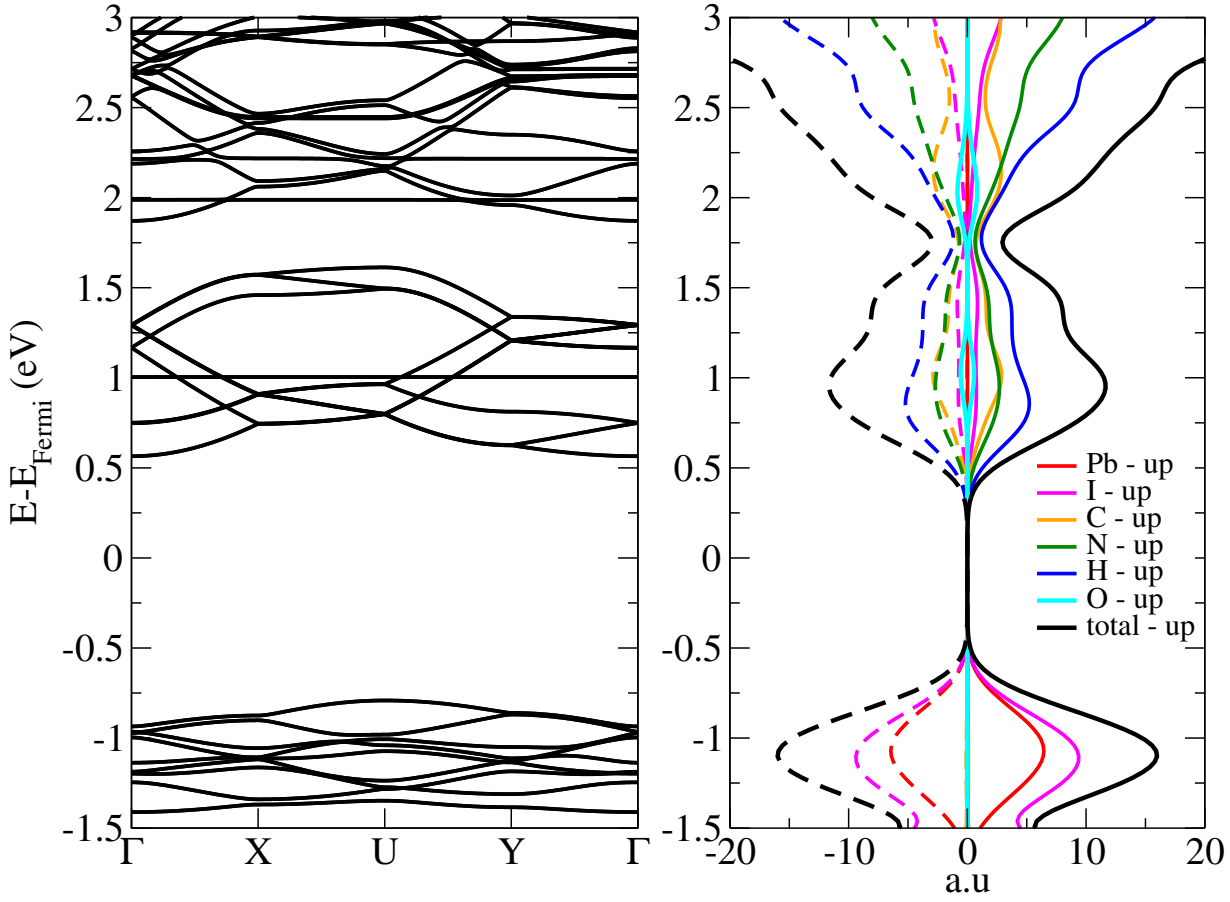

FIG. S3. From left to right: electronic band structure and the corresponding projected density of states (PDOS) for the MA covered $MAPbI_3$/caffeine system presented in Figure S1.