Supplementary Information (SI) for Inorganic Chemistry Frontiers.

Supplementary Information

Insights into the role of iron coordination in the enhanced photoactivity of $MAPbI_3$/iron oxides heterojunctions†

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Table. S1 Crystal structure and lattice parameters in this paper.

Compound	Symmetry	Lattice constants					
		Lattice parameter(Å)			Lattice angel (°)		
		a	b	c	α	β	γ
$CH_3NH_3PbI_3$	$Pm\bar{3}m$	6.29	6.29	6.29	90	90	90
α-Fe_2O_3	$R\bar{3}c$	5.03	5.03	13.75	90	90	120
γ-Fe_2O_3	$Fd\bar{3}m$	8.33	8.33	8.33	90	90	90
TiO_2	$I4_1amd$	3.78	3.78	9.49	90	90	90

Table. S2 The interfacial distance between terminals on different surfaces (Å).

Compound	MAI	PbI
α-Fe_2O_3-Fe_{o1}	2.60	2.00
α-Fe_2O_3-Fe_{o2}	2.60	2.50
γ-$Fe_2O_3Fe_t$	2.66	2.60
γ-Fe_2O_3-Fe_o	2.61	2.32
TiO_2	3.17	2.45

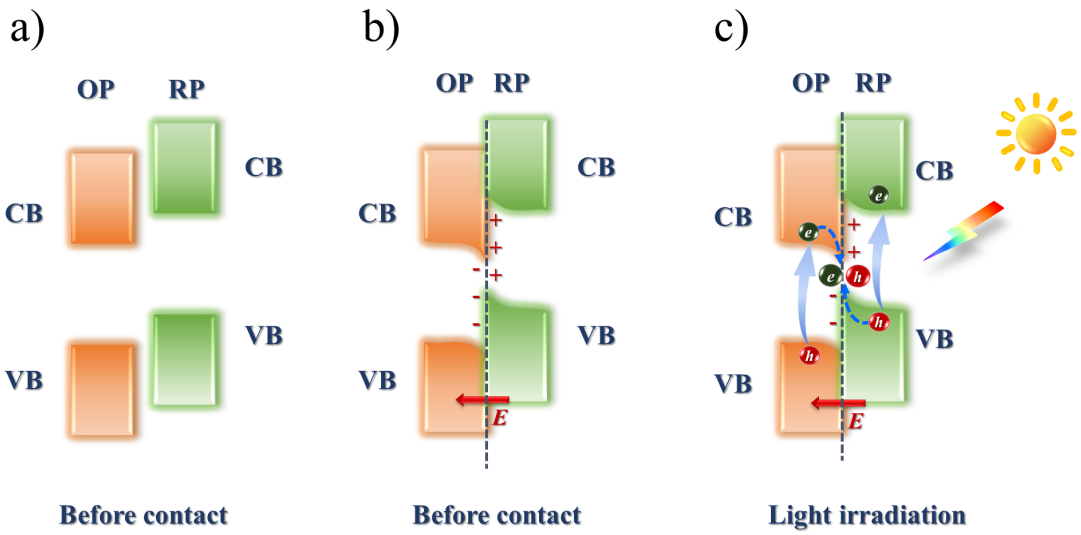

Fig. S1 Charge-transfer processes in an S-scheme heterojunction: (a) before contact, (b) after contact; and (c) photogenerated charge carrier transfer under light irradiation.

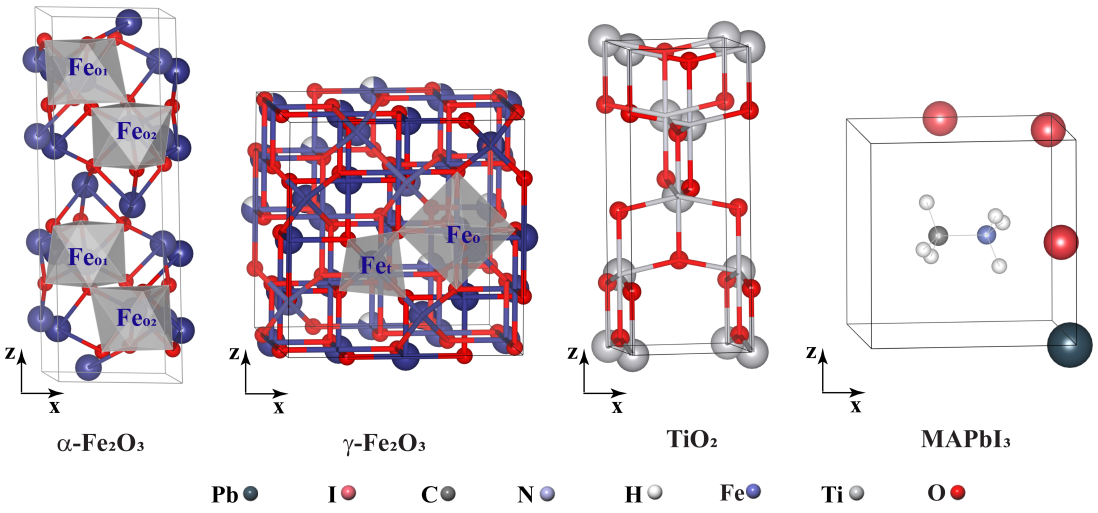

Fig. S2 Illustration of crystal structures.

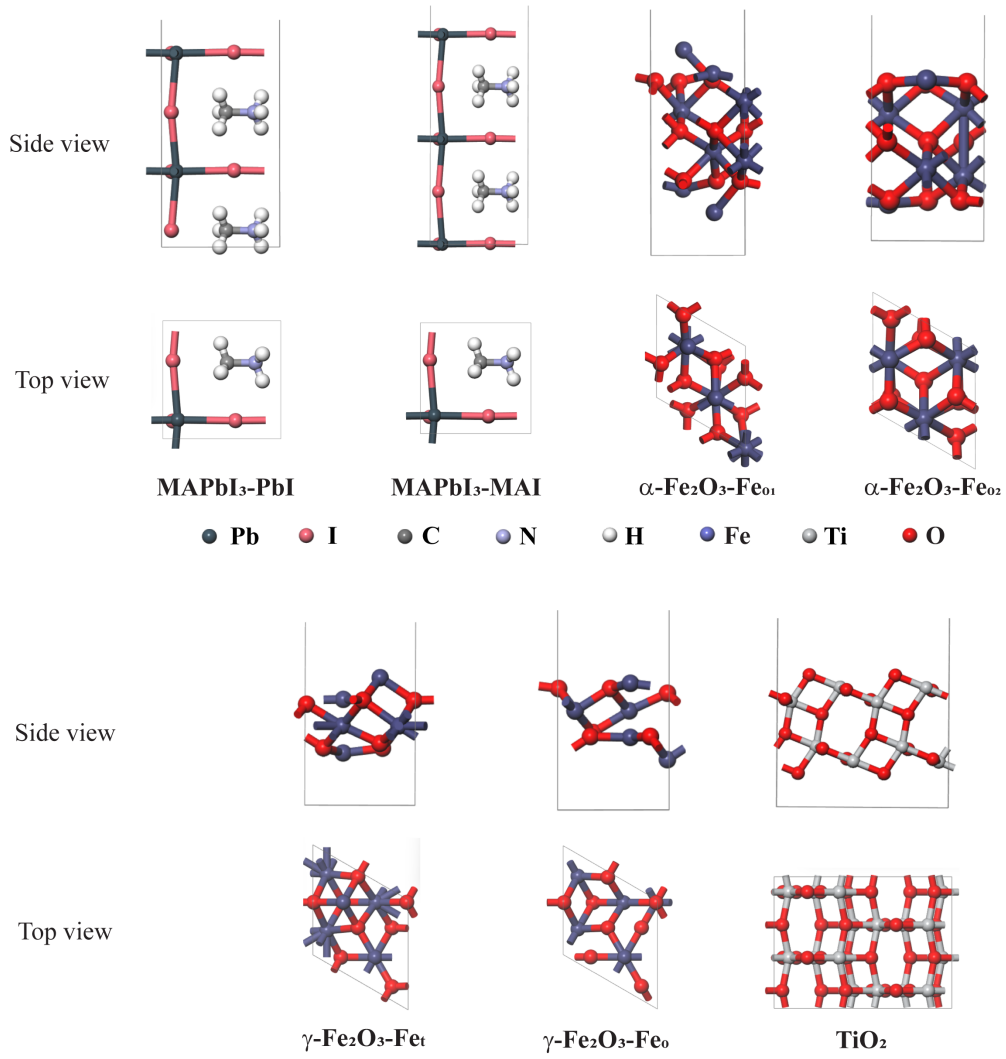

Fig. S3 The optimized surface structures.

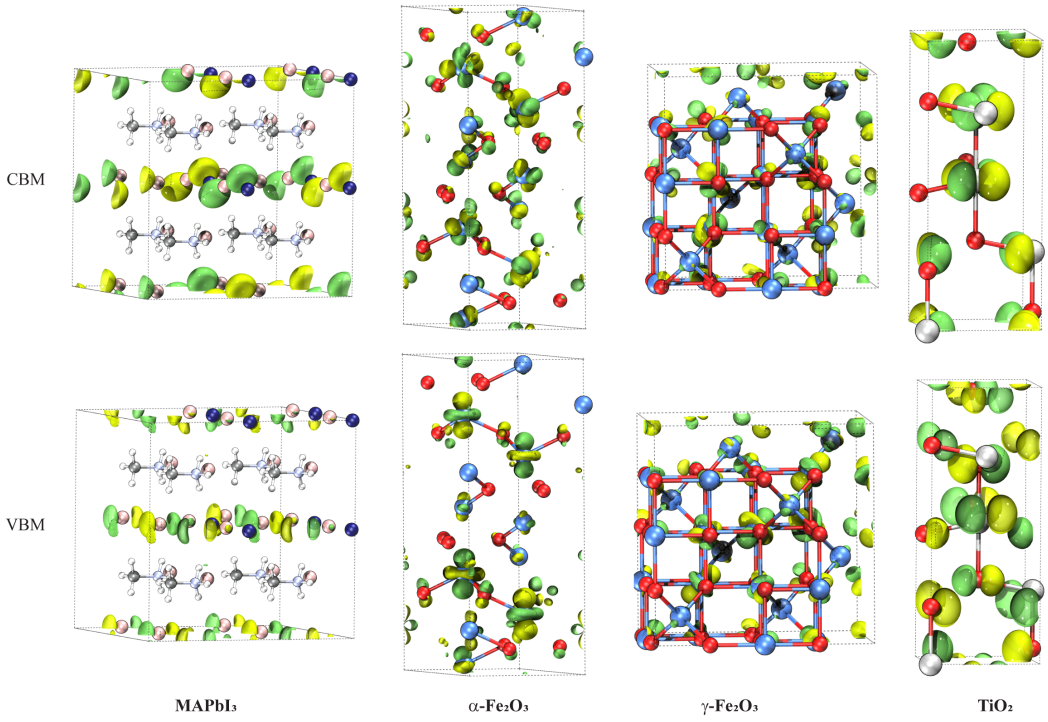

Fig. S4 The valence band maxima (VBM) and conduction band minima (CBM) charge densities in the bulk geometry. The positive electron density is shown in green, the negative electron density is shown in yellow, and the value of the isosurface is 0.05 e Å^{-3}.

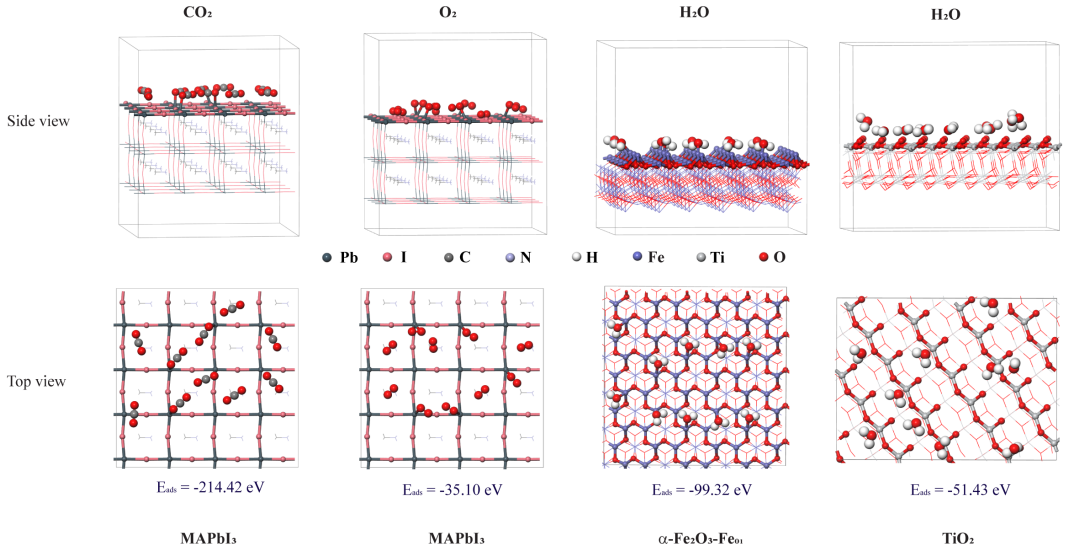

Fig. S5 Adsorption of ten carbon dioxide and oxygen molecules on $MAPbI_3$ (001) surface, and adsorption of ten water molecules on α-Fe_2O_3 (001) and TiO_2 (101) surface.