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

Enhancing the Stability of Perovskite by Constructing Heterojunction of Graphene/$MASnI_3$

Zhihua Hu, [a] Yanli Zeng,*[b] Xiaoyan Li,[a] and Lingpeng Meng*[a]

[a] College of Chemistry and Material Science, Hebei Normal University, Shijiazhuang, 050024 China

[b] National Demonstration Center for Experimental Chemistry Education, Hebei Normal University, Shijiazhuang, 050024 China

Table S1 Atomic Bader charge before and after the adsorption of H_2O molecule.

SnI_2-surface	Sn2		I4		H_2O	
Sn site	before	after	before	after	before	after
Charge	13.06	12.98	7.49	7.53	8.01	7.97
net Charge	0.94	1.02	-0.49	-0.53	-0.01	0.03
MAI-surface	I15		$CH_3NH_3^+$		H_2O	
$CH_3NH_3^+$ site	before	after	before	after	before	after
Charge	7.61	7.60	14.25	14.24	8.01	8.04
net Charge	-0.61	-0.60	0.75	0.76	-0.01	-0.04
heterojunction	graphene				H_2O	
top C site	before		after	before		after
Charge	120.02		120.01	8.01		8.01
net Charge	-0.02		-0.01	-0.01		-0.01

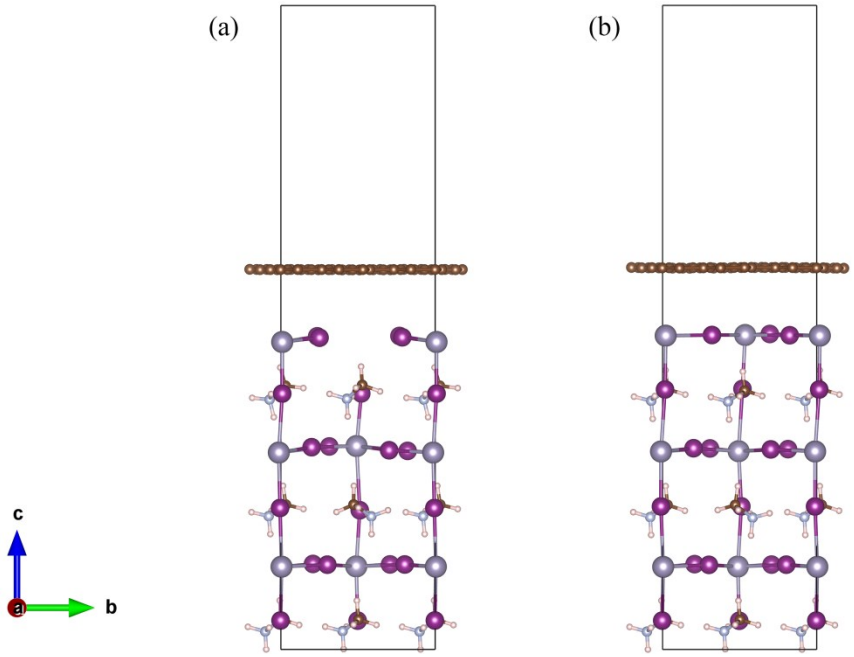


Figure S1 Configurations of heterojunctions with vacancy defect in perovskite sufaces. (a) Sn vacancy defect V_{Sn}; (b) I vacancy defect V_I.

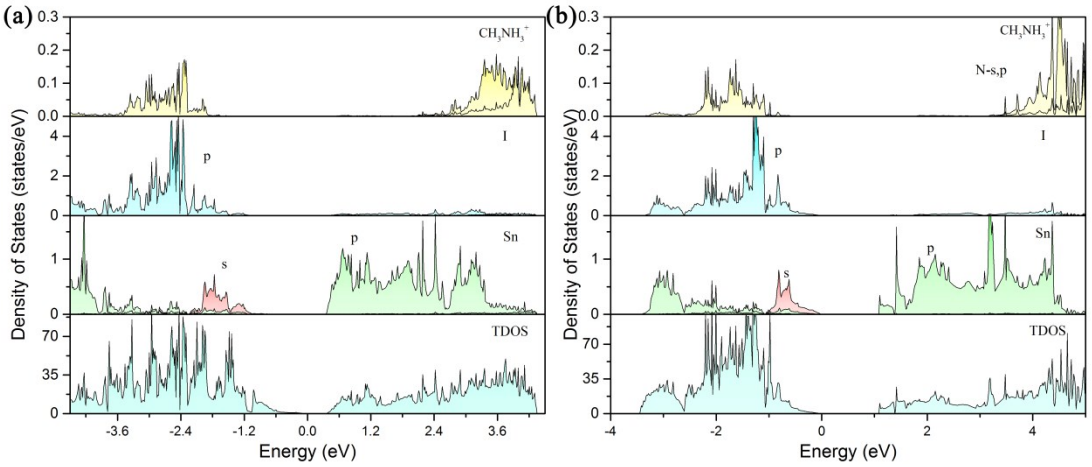
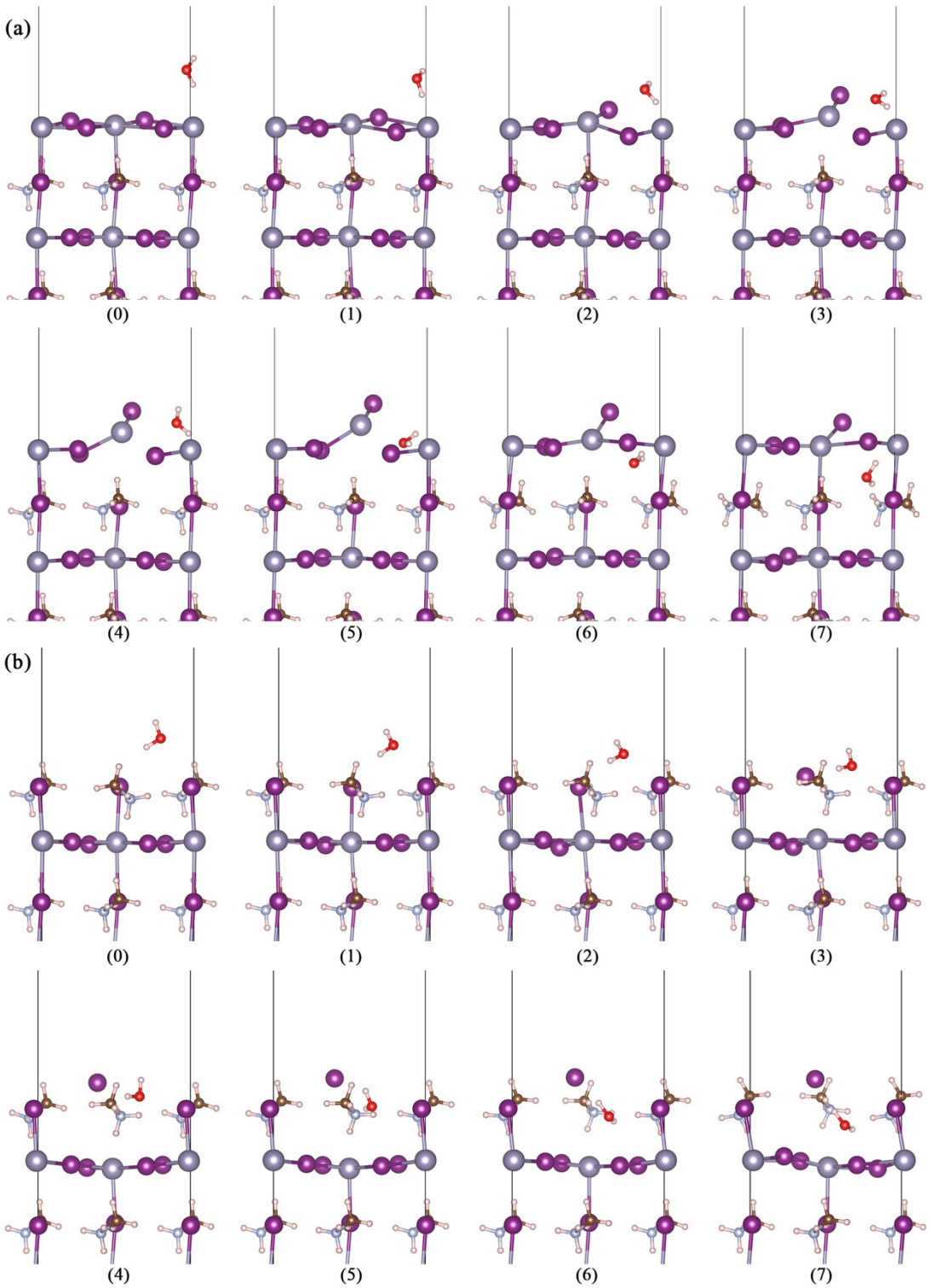


Figure S2 Total and projected DOS of SnI_2-terminated (a) and MAI-terminated (b) surface of $MASnI_3$.


(a)
(0)
(1)
(2)
(3)
(4)
(5)
(6)
(7)
(b)
(0)
(1)
(2)
(3)
(4)
(5)
(6)
(7)

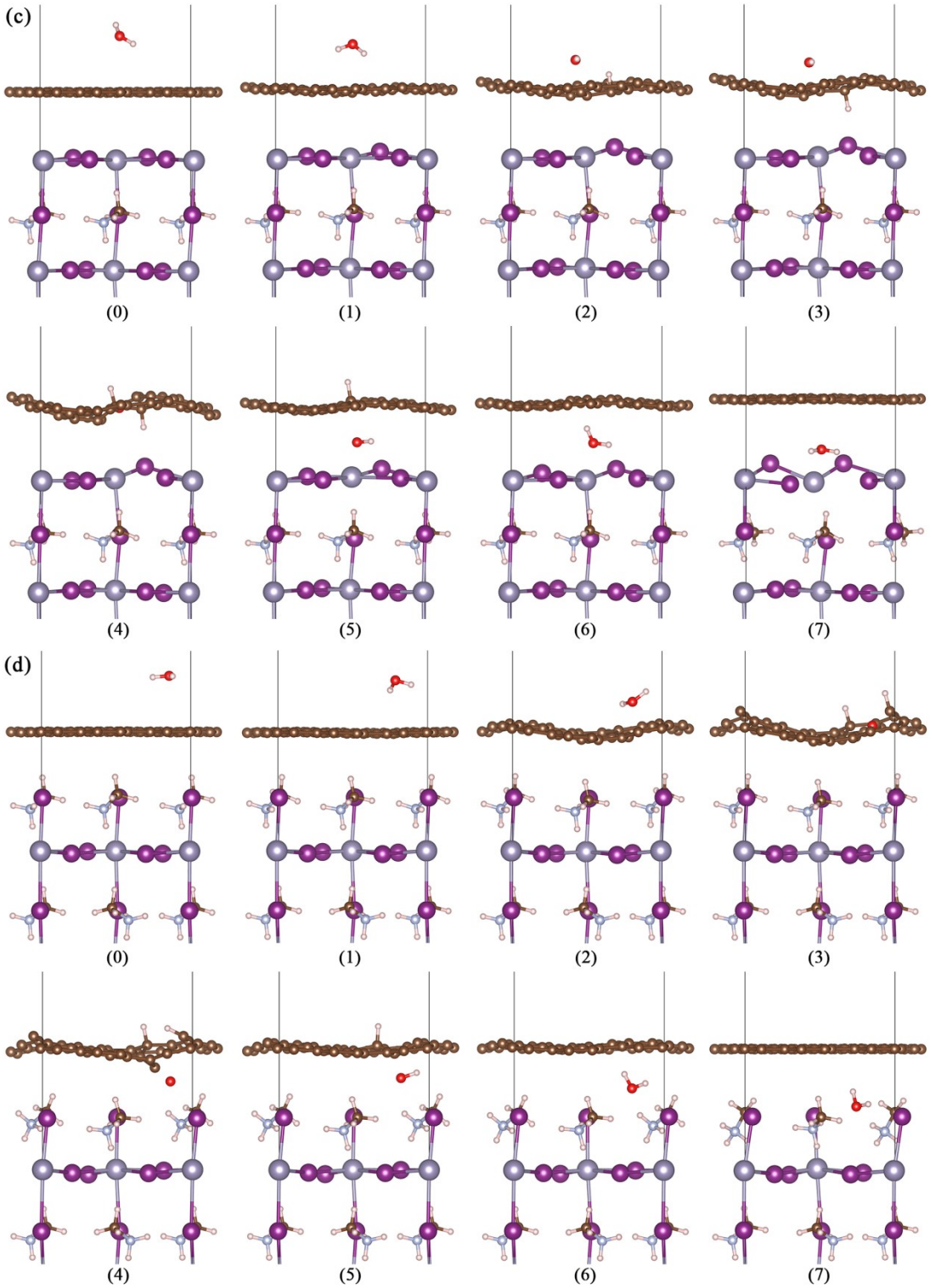


Figure S3 Configurations at the points of diffusion path of H_2O passing through the surface. (a) SnI_2-terminated surface of $MASnI_3$; (b) MAI-terminated surface of $MASnI_3$; (c) graphene/SnI_2 heterojunction; (d) graphene/MAI heterojunction.