

Supplementary Material

Boosting the Adsorption and Sensing Performance of MoS₂ for SF₆ Decomposition Gases by Non-Metal Atom Doping: A DFT Study

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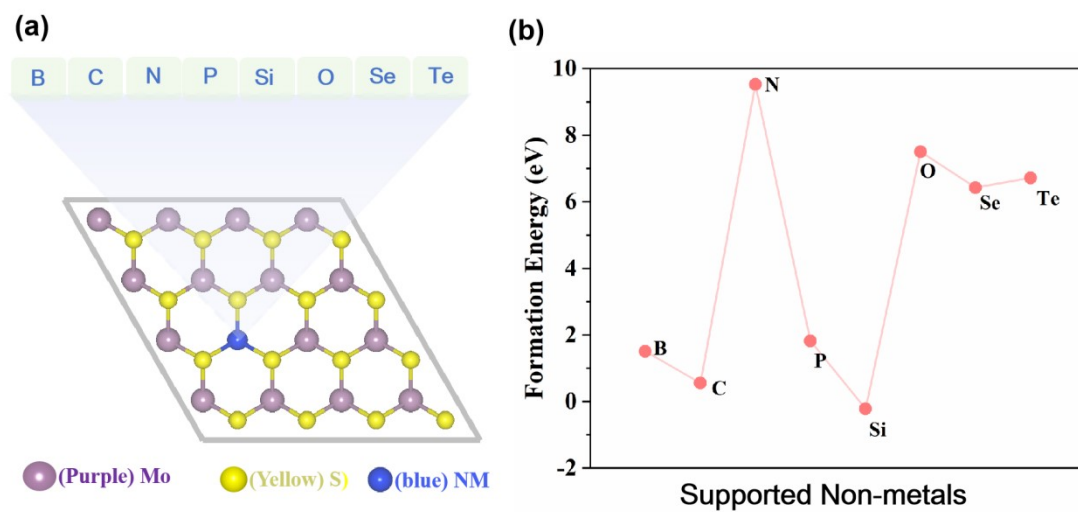


Fig. S1. (a) Structure of NM atoms replacing Mo sites in monolayer MoS₂; (b) Formation energies of NM atoms substitution at Mo sites in monolayer MoS₂.

Table S1. Comparison of adsorption energies for SF₆ Decomposition Gases.

System	Gas	E _{ad} (eV)	Ref.
B@MoS ₂	H ₂ S	-1.66	This work
	SO ₂	-1.22	
	SOF ₂	-0.98	
	SO ₂ F ₂	-0.49	
C@MoS ₂	H ₂ S	-1.62	This work
	SO ₂	-1.15	
	SOF ₂	-1.00	
	SO ₂ F ₂	-0.44	
N@MoS ₂	H ₂ S	-0.46	This work
	SO ₂	-0.68	
	SOF ₂	-0.51	
	SO ₂ F ₂	-0.39	
P@MoS ₂	H ₂ S	-0.55	This work
	SO ₂	-0.75	
	SOF ₂	-0.44	
	SO ₂ F ₂	-0.39	
Si@MoS ₂	H ₂ S	-1.67	This work
	SO ₂	-0.93	
	SOF ₂	-0.64	
	SO ₂ F ₂	-0.74	
P@MoS ₂	H ₂ S	-0.367	1
Pd@MoSe ₂	H ₂ S	-1.234	2
	SO ₂	-1.348	
	SOF ₂	-1.193	
	SO ₂ F ₂	-0.654	
Rh@MoSe ₂	H ₂ S	-1.187	2
	SO ₂	-1.665	
	SOF ₂	-1.441	
	SO ₂ F ₂	-1.600	
MoS ₂	SO ₂	-0.233	3
P@MoS ₂	SO ₂	-0.514	3
Cl@MoS ₂	SO ₂	-0.362	3
Ge@MoS ₂	SO ₂	-0.883	3
Se@MoS ₂	SO ₂	-0.183	3
Ir@HfS ₂	H ₂ S	-1.22	4
	SOF ₂	-0.79	
	SO ₂ F ₂	-0.45	
Pt@HfS ₂	H ₂ S	-0.95	5

Sc@MoS ₂	SOF ₂	-0.43	6
	H ₂ S	-1.10	
	SO ₂	-3.21	
	SOF ₂	-4.69	
	SO ₂ F ₂	-7.09	
PtSe ₂	H ₂ S	-0.23	7
	SO ₂	-0.29	
	SOF ₂	-0.23	
	SO ₂ F ₂	-0.26	
Ir@MoS ₂	H ₂ S	-2.323	8
	SO ₂	-1.757	
	SOF ₂	-1.492	
Cu@MoTe ₂	SO ₂	-1.02	9
	SOF ₂	-0.68	
	SO ₂ F ₂	-0.29	
Au@MoS ₂	H ₂ S	-0.96	10
	SO ₂	-1.18	
Pt@WTe ₂	SO ₂	-1.36	11
	SOF ₂	-1.17	
Ni@MoS ₂	H ₂ S	-1.319	12
	SO ₂	-0.823	

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