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SUPPLEMENTARY INFORMATION

Electronic and optical properties of MoS_2/α-Fe_2O_3(0001) heterostructure: a first-principles investigation

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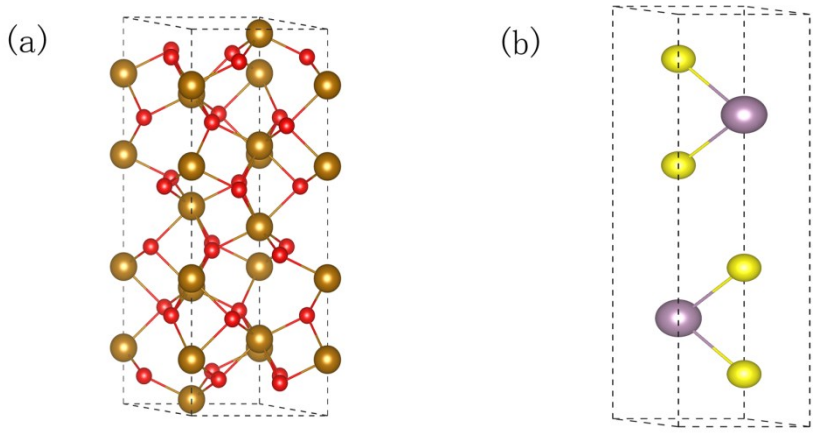

Fig. S1 Crystal structure of (a) pure hematite and (b) molybdenum disulfide.

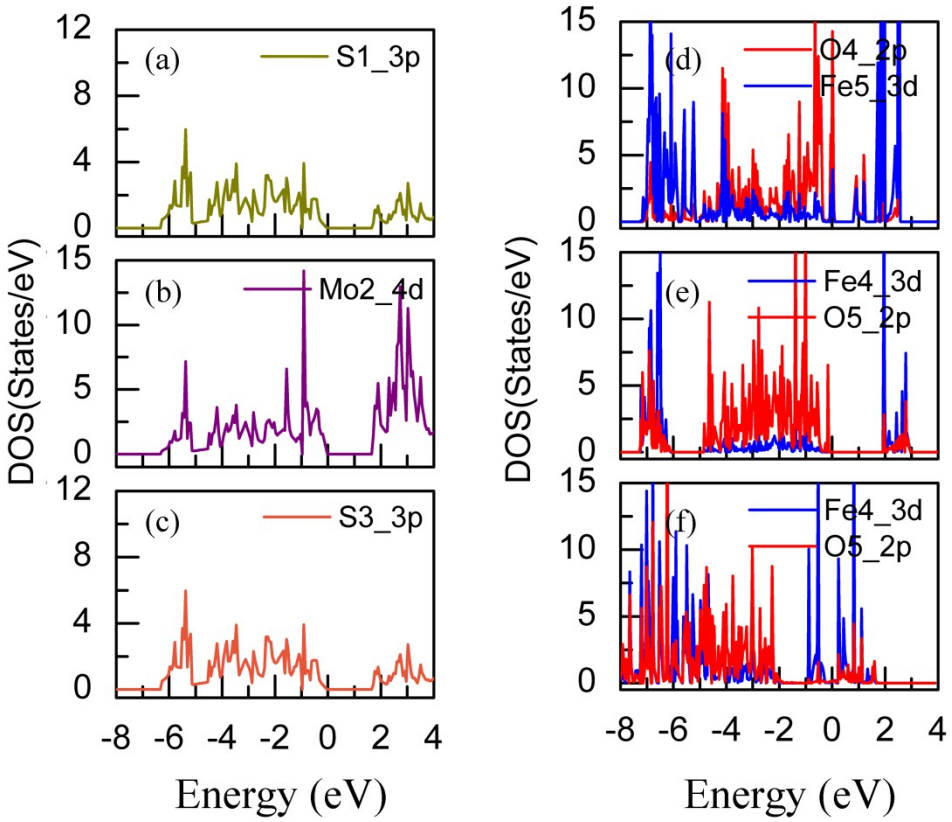

Fig. S2 The layer resolved density of states (DOS) for (a, b, c) the isolated MoS_2 film, (d) O_3–Fe–Fe–R, (e) Fe–O_3–Fe–R, and (f) Fe–Fe–O_3–R surface.

Table S1 The lattice parameters and bandgaps of bulk MoS_2 obtained by PBE-D simulation and the available experimentally measured data.

	a=*b* (Å)	c (Å)	E_g (eV)
Expt.	3.16[1, 2]	12.29[1, 2]	1.20[3]
Calc.	3.18[4]	12.43[4]	0.95[4]
This work	3.19	12.49	0.94

Table S2 The total energy of MoS_2/α-Fe_2O_3 (0001) heterostructure with different in-plane lattice parameter

	Lattice parameters a=b (Å)	Total energy (eV)
MoS_2/O_3–Fe–Fe–R	5.07	-207.83528293
	5.12	-208.16406543
	5.18	-208.37617414
	5.23	-208.39028533
	5.28	-208.25469251
	5.33	-208.03863949
	5.39	-206.35441179
	5.44	-207.15890369
	5.50	-206.54806926
MoS_2/Fe–O_3–Fe–R	5.07	-191.53773096
	5.12	-191.69824521
	5.18	-190.98289629
	5.23	-192.71168897
	5.28	-191.69874432
	5.33	-190.15941566
	5.39	-191.47392496
	5.44	-192.00033671
	5.50	-191.33192446
MoS_2/Fe–Fe–O_3–R	5.07	-184.88989304
	5.12	-185.27932991
	5.18	-185.58978295
	5.23	-185.69331388
	5.28	-185.64442385
	5.33	-185.51309613
	5.39	-184.53757827
	5.44	-184.97853721
	5.50	-183.52187112

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