Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Gas adsorption on MoS_2/WS_2 in-plane heterojunction and the I-V response: A first principles study

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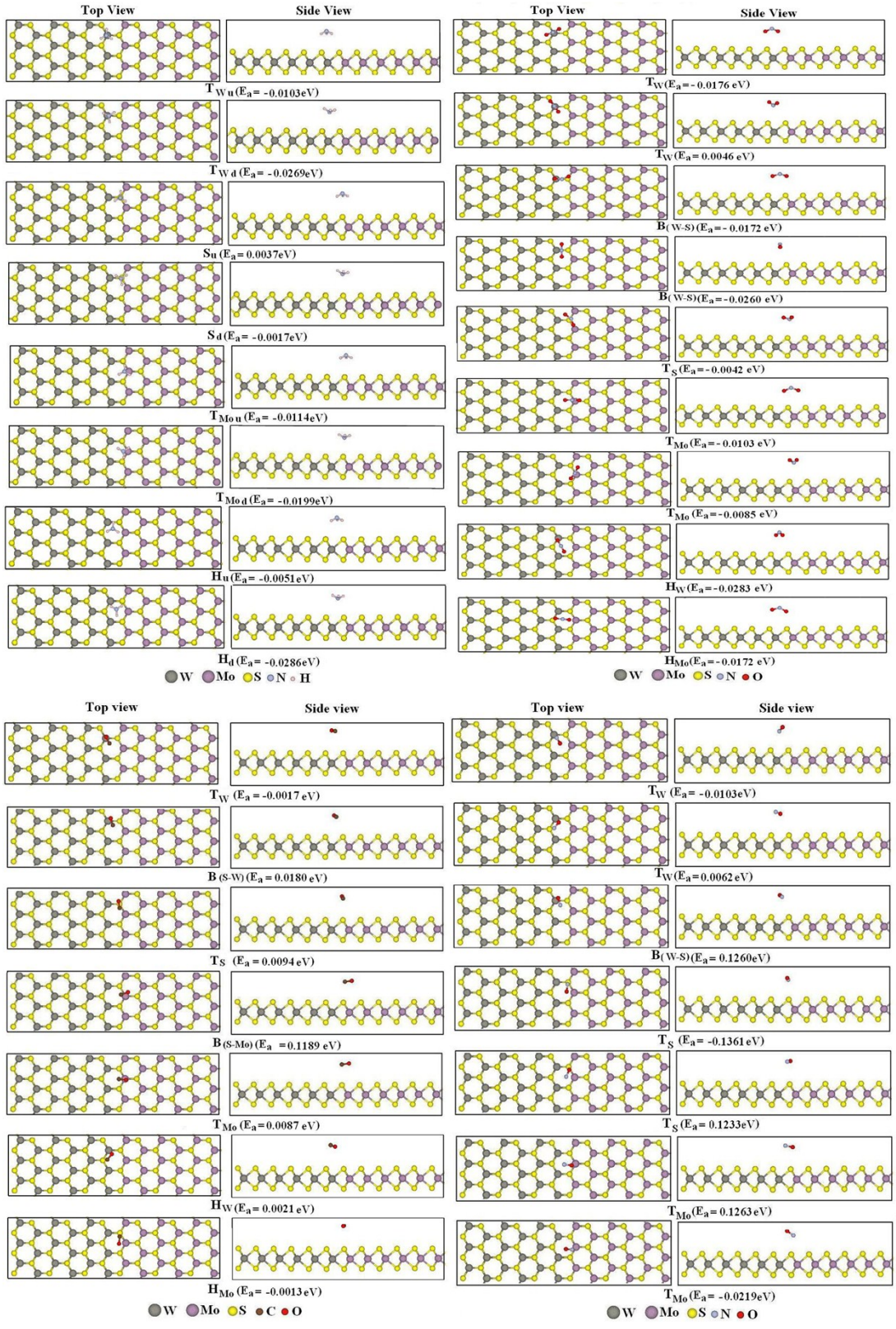
Section 1. The molecules adsorption configurations



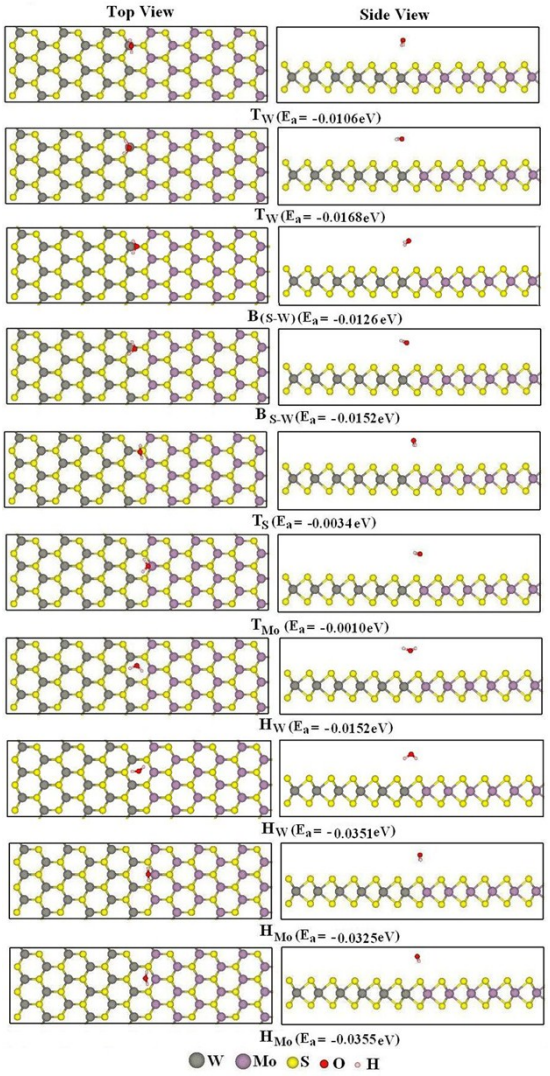


Figure S1. The involved geometry structures used to determine the favorable molecules adsorption configurations.

Section 2. The Molecules adsorbed on WS_2 site.

Beside the molecules adsorbed on the interface, we carefully check the configurations of the molecules adsorbed on the WS_2 site and list the adsorption energies (Ea), equilibrium height (d), and charge transfer (ΔQ) in Table S1. We note that both the adsorption energies and the charge transfer behavior of the molecules adsorbed on WS_2 are similar to that adsorbed on the interface of heterojunciton. Moreover, the total density of states of the molecules adsorbed on the WS_2 site are also shown in Figure S2, which have little discrepancy with that adsorbed on the

interface. This may indicate the adsorption sites have negligible impact on the electronic structure of molecules adsorbed on the heterojunciton.

Table S1. Calculated adsorption energies (Ea), equilibrium height (d), and charge transfer (ΔQ) of the molecules adsorbed on WS_2 site using PBE with vdW correction.

Molecule	Ea (eV)	d (Å)	ΔQ (e)
CO	-0.0999	3.2861	-0.0083
H_2O	-0.1592	2.6063	-0.0139
NH_3	-0.1595	2.9201	0.0228
NO	-0.1274	3.0192	-0.0466
NO_2	-0.1644	3.1099	-0.0518

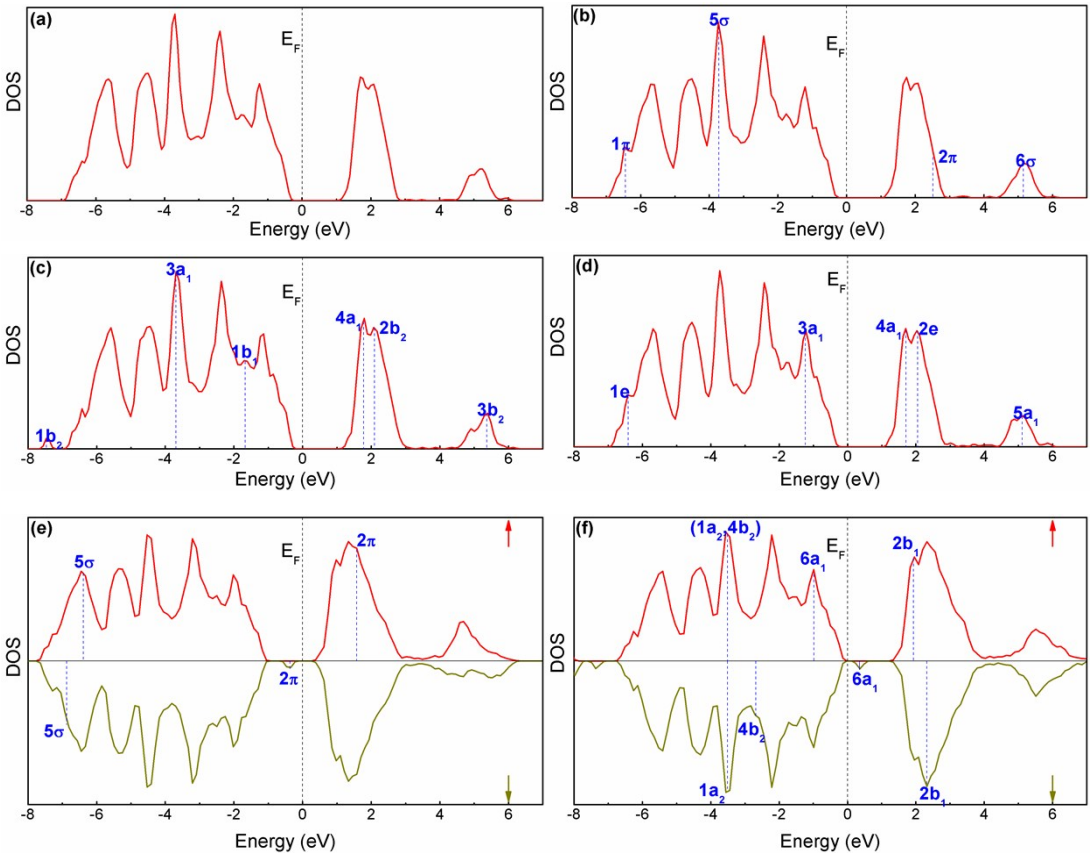


Figure S2. (a) Total DOS of heterojunction and with each gas molecule adsorption on WS_2 site (b) CO, (c)H2O, (d)NH3, (e) NO and (f)NO2. The blue dotted lines show the positions of the molecular orbitals. The Fermi level is shifted to zero indicated by the black dashed lines.

Section 3. Band alignment in the lateral WS_2–MoS_2 heterojunction

We have calculated the band alignments by using the macroscopic averaging method[1]. The electrostatic potential is chosen as a reference and the change of the average electrostatic potential through the interface is obtained by calculating the WS_2-MoS_2 heterojunction. The valence-band-maximum (VBM) and the conduction-band-minimum (CBM) of the two semiconductors with respect to the electrostatic potential are calculated by using their individual monolayer unit cell. The calculated results are shown in Figure S3. We can see that the VBM and CBM of WS_2 are respectively 0.14 eV and 0.39 eV, which are both higher than those of MoS_2, indicating that the WS2-MoS2 heterojunction has a type II band alignment character.

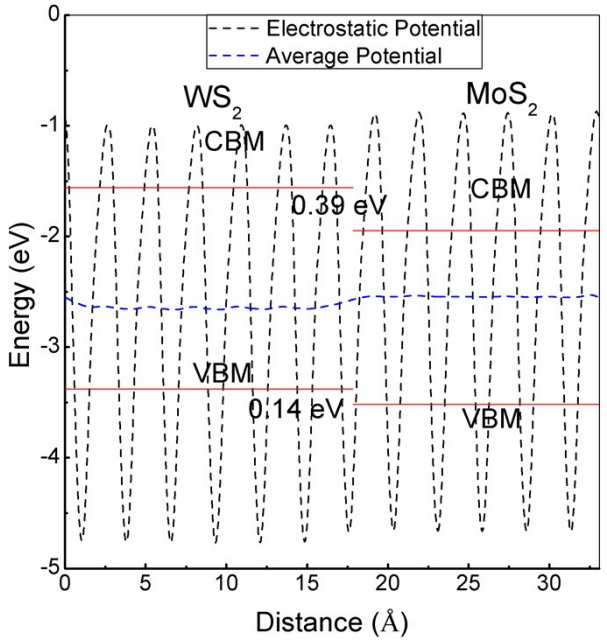


Figure S3. Band alignment in the lateral WS_2–MoS_2 heterojunction

Reference:

1. A. Baldereschi, S. Baroni, and R. Resta, Phys. Rev. Lett. 1988, 61, 734.