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 (E$_a$), 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 heterojunctiton. 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 heterojunction.

**Table S1.** Calculated adsorption energies (Ea), equilibrium height (d), and charge transfer (ΔQ) of the molecules adsorbed on WS₂ site using PBE with vdW correction.

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Ea (eV)</th>
<th>d (Å)</th>
<th>ΔQ (e)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO</td>
<td>-0.0999</td>
<td>3.2861</td>
<td>-0.0083</td>
</tr>
<tr>
<td>H₂O</td>
<td>-0.1592</td>
<td>2.6063</td>
<td>-0.0139</td>
</tr>
<tr>
<td>NH₃</td>
<td>-0.1595</td>
<td>2.9201</td>
<td>0.0228</td>
</tr>
<tr>
<td>NO</td>
<td>-0.1274</td>
<td>3.0192</td>
<td>-0.0466</td>
</tr>
<tr>
<td>NO₂</td>
<td>-0.1644</td>
<td>3.1099</td>
<td>-0.0518</td>
</tr>
</tbody>
</table>

**Figure S2.** (a) Total DOS of heterojunction and with each gas molecule adsorption on WS₂ 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 WS$_2$–MoS$_2$ heterojunction has a type II band alignment character.

![Figure S3. Band alignment in the lateral WS$_2$–MoS$_2$ heterojunction](image)

Reference: