

Electronic Supporting Information

Interaction between H₂O, N₂, CO, NO, NO₂ and N₂O molecules and the defective

WSe₂ monolayer

Dongwei Ma^{1,*}, Benyuan Ma², Zhiwen Lu², Chaozheng He^{2,*}, Yanan Tang^{3,*},
Zhansheng Lu⁴ and Zongxian Yang⁴

¹*School of Physics, Anyang Normal University, Anyang 455000, China*

²*Physics and Electronic Engineering College, Nanyang Normal University, Nanyang
473061, China*

³*College of Physics and Electronic Engineering, Zhengzhou Normal University,
Zhengzhou, 450044, China*

⁴*College of Physics and Materials Science, Henan Normal University, Xinxiang
453007, China*

*Corresponding author. E-mail: dwmachina@126.com (Dongwei Ma).

*Corresponding author. E-mail: hecz2013@nynu.edu.cn (Chaozheng He).

*Corresponding author. E-mail: yntang2010@163.com (Yanan Tang).

Table S1. The nearest atomic distance (d in Å) between the adsorbed molecule and the V_{Se} surface for the physisorption state. From the reference (*Dalton Transactions, 2008* (21): 2832-2838), the sum of the covalent radii of C, N, or O and W (Se) atoms is about 2.3 (1.9) Å, and that of H and W (Se) atoms is about 1.9 (1.5) Å.

molecule	H ₂ O	N ₂	CO	NO	NO ₂	N ₂ O
d	3.17	3.95	3.71	3.36	3.35	3.50

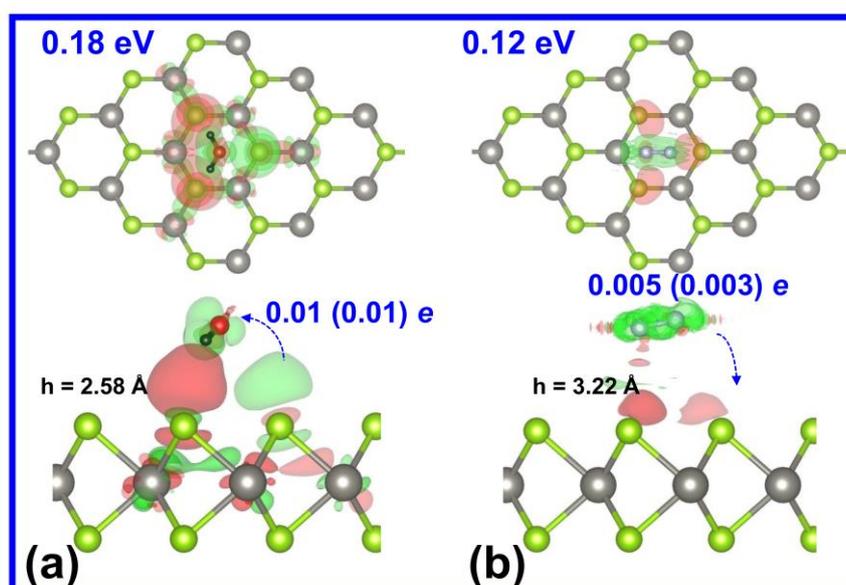


Fig. S1. The top and side views of the pristine WSe₂ monolayer with the physisorbed H₂O (a) and N₂ (b) molecules. The adsorption energy, the number the transferred electrons, and the height of the adsorbed molecule with respect to the upper Se atomic plane are given. The isosurfaces for the CDD are 2×10^{-4} and 1×10^{-4} e bohr⁻³, respectively, for the adsorption of the H₂O and N₂ molecules. The red and green regions represent the electron accumulation and depletion, respectively.

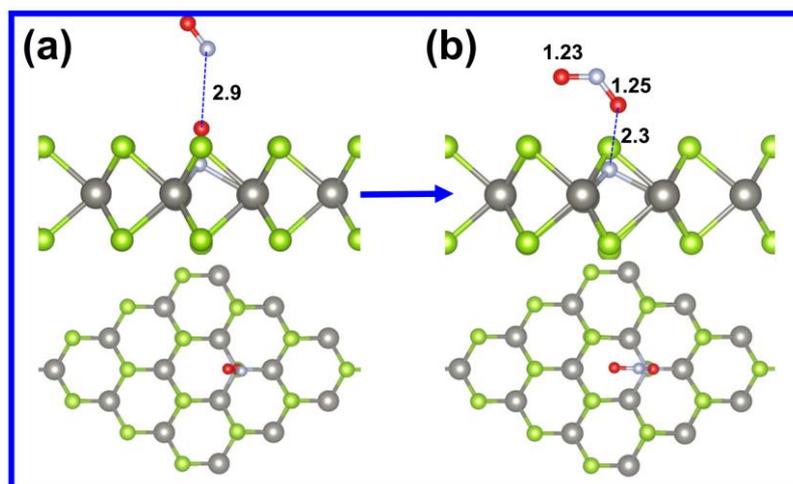


Fig. S2. (a) A NO molecule is put above the NO molecule doped WSe₂ monolayer. (b) After structural optimization for the configuration in (a), the NO molecule can combine with the exposed O atom to form a N-doped WSe₂ monolayer with an adsorbed NO₂ molecule.

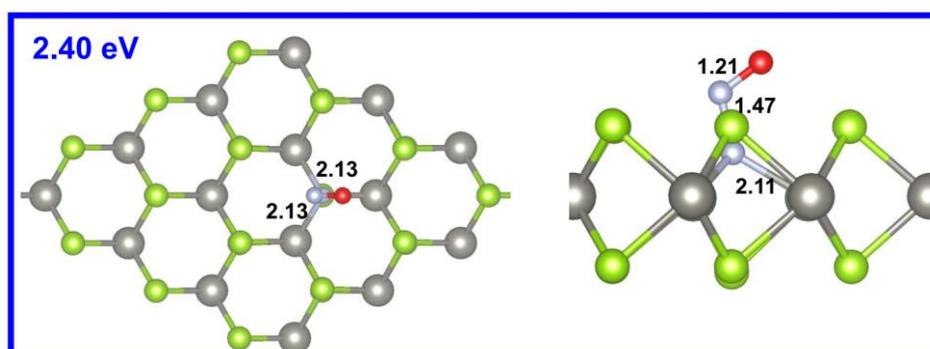


Fig. S3. The top and side views of the N₂O molecule adsorption on VSe with the N atom occupying the Se vacancy site. The adsorption energy for this configuration is 2.40 eV.

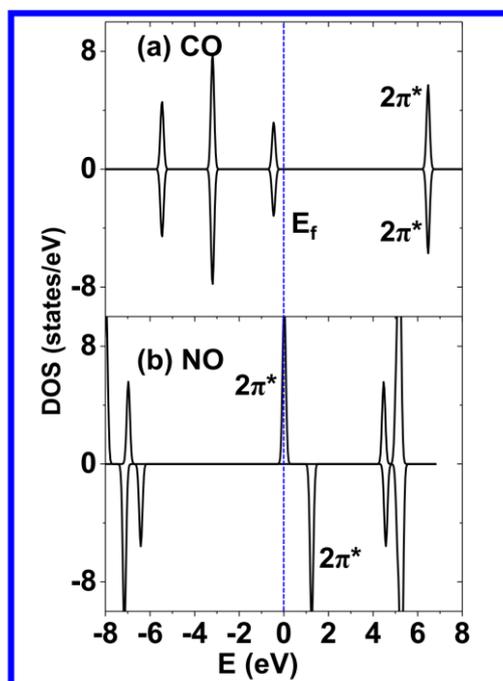


Fig. S4. The spin-polarized TDOS of the free CO (a) and NO molecules (b). The $2\pi^*$ levels near the E_f are marked.

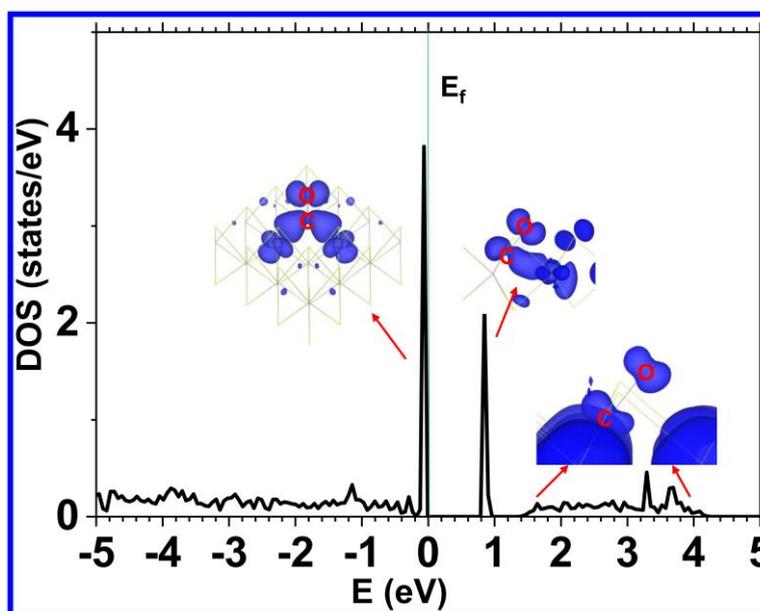


Fig. S5. The LDOS projected on the adsorbed CO for the MC state. The insets show the partial charge densities for the electronic states within -0.2 to 0.0 eV (in 0.003 e/bohr³), within 0.7 to 1.0 eV (in 0.003 e/bohr³), and within 1.4 to 4.0 eV (in 0.03 e/bohr³). The vertical line denotes the Fermi level.

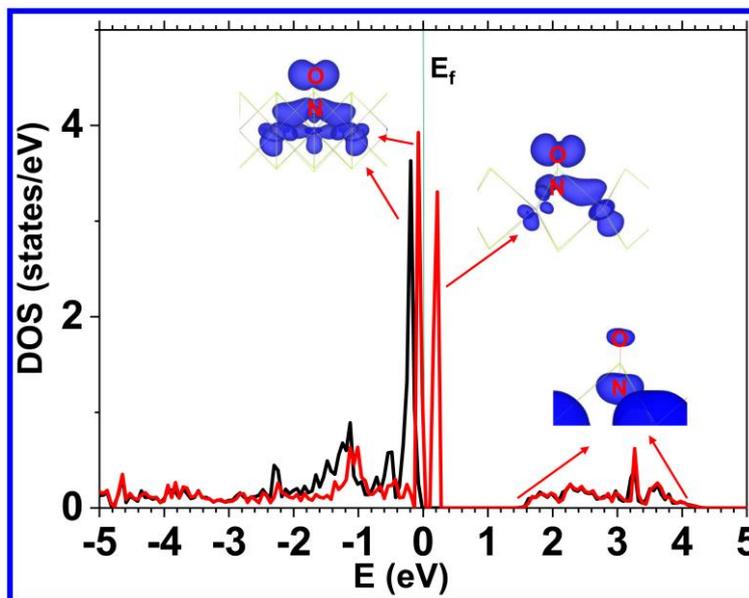


Fig. S6. The LDOS projected on the adsorbed NO for the MC state. The insets show the partial charge densities for the electronic states within -0.4 to 0.0 eV (in 0.006 e/bohr^3), within 0 to 0.2 eV (in 0.003 e/bohr^3), and within 2.0 to 4.0 eV (in 0.03 e/bohr^3). The vertical line denotes the Fermi level. The black and red lines indicate the spin-up and spin-down states, respectively.