Supporting Information

for

Free-radical gases on two-dimensional transition-metal disulfides (XS_2, X = Mo/W): robust half-metallicity for efficient nitrogen oxide sensors

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Additional computational data

Method

The spin-polarized structural relaxation and electronic property calculations were carried out using density functional theory (DFT) with the Perdew–Burke–Ernzerhof (PBE) generalized gradient approximation [1] exchange–correlation potential as implemented in the Vienna ab initio simulation package (VASP) [2-4]. A dispersion correction of the total energy (DFT-D3 method) [5] was used to incorporate the long-range van der Waals interactions. In addition to MoS_2, and WS_2, we expand our 2D material to GaS, GaSe, SnS, SnSe, WSe and Bi_2Se_3 (Figure S1). A cut-off energy of 500 eV for the plane-wave basis set and a Monkhorst–Pack mesh [6] of 7 × 7 × 1 for the unit cell, 3 × 3 × 1 for the 3 × 3 supercell, and 3 × 3 × 1 for the 6 × 6 supercell for the Brillouin zone integration are employed to find the most favorable adsorption sites for NO and NO_2. For simplicity, only the PDOS of a single NO gas adsorption on unit cell surface is given in Figure S1. The unit cell for a single NO_2 adsorption is not incorporated in order to guarantee a certain distance between two neighbouring NO_2 molecules (Figure S2).

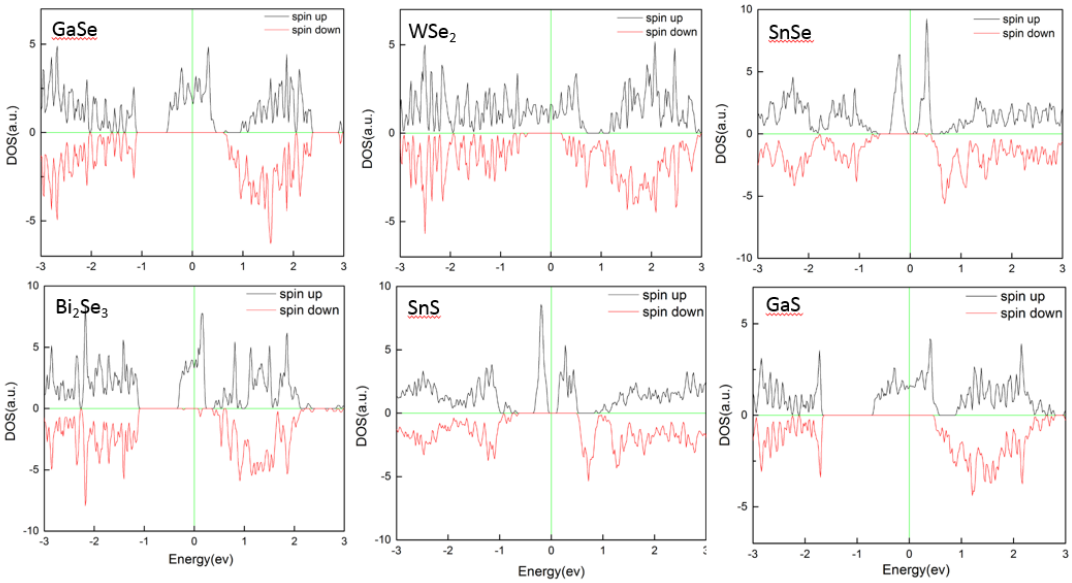

Figure S1: Total density of states (DOS) of NO adsorbed GaSe, WSe_2, SnSe, Bi_2Se_3, SnS and GaS. The Fermi level is indicated by the green line.

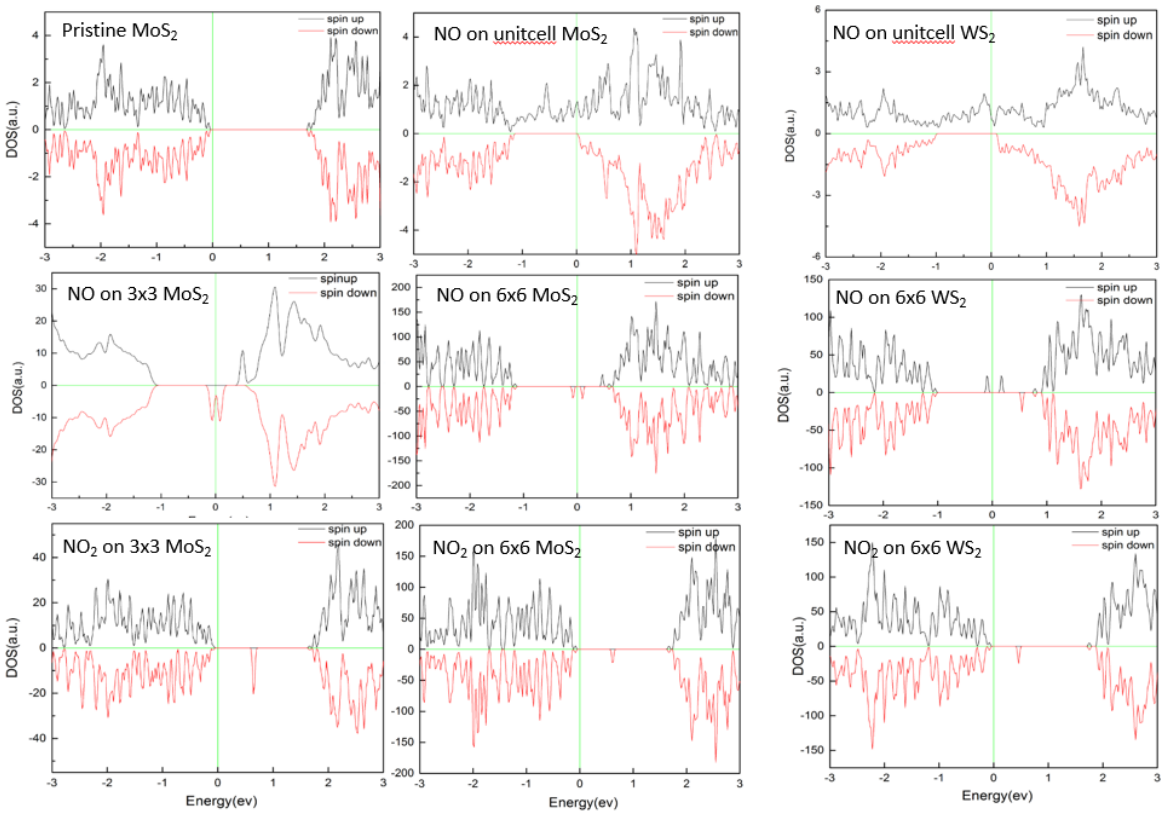

Figure S2: Total density of states (DOS) of the pristine 2D MoS_2 unit cell, 3 × 3 supercell and 6 × 6 MoS_2 supercell and with and with NO*x* (*x* = 1, 2) adsorbed. The Fermi level is indicated by the green line.

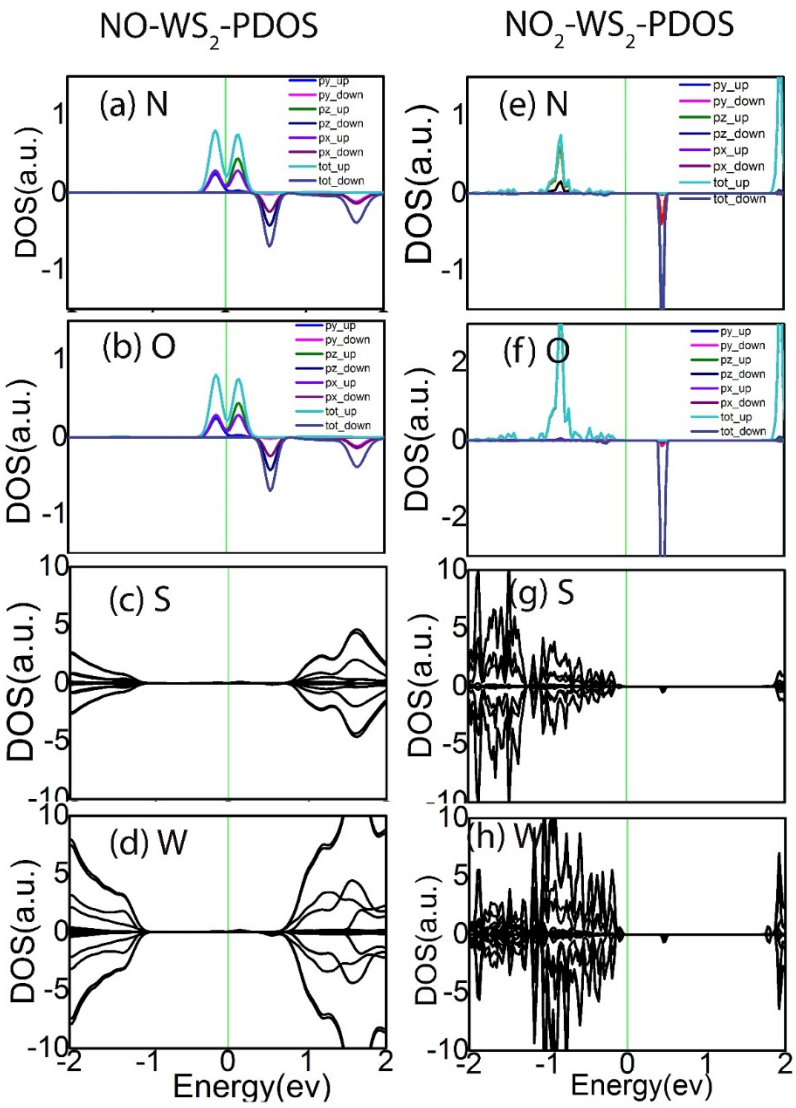

Figure S3: The N, O, W and S PDOS of WS_2 with (a–d) adsorbed NO and with (e–h) adsorbed NO_2. The Fermi level is indicated by the green line.

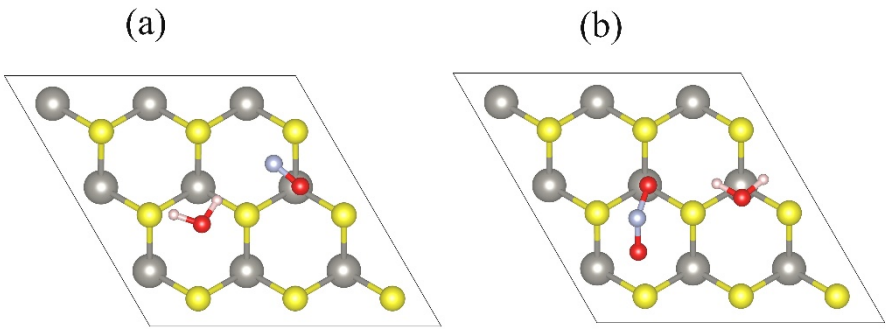

Figure S4: WS_2 with (a) adsorbed NO and with (b) adsorbed NO_2 in humid environment. The white, red, yellow, grey, dark grey balls represent H, O, S, N, W atoms, respectively.

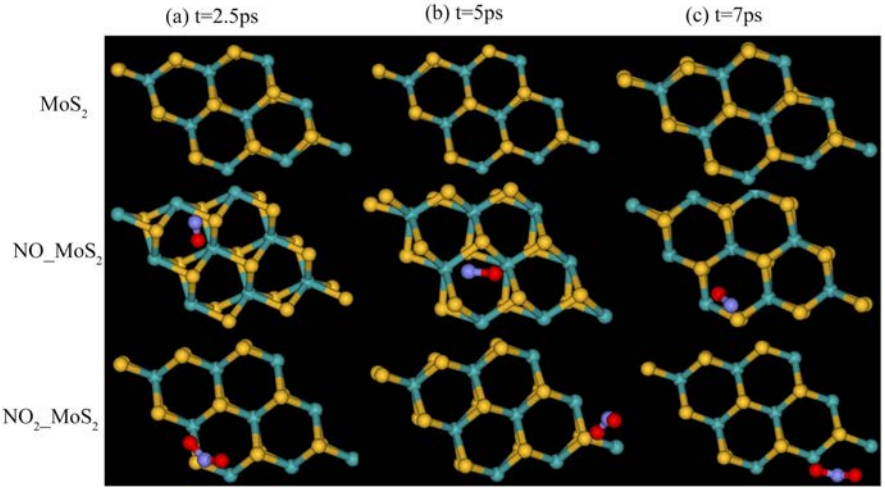

Figure S5: The thermodynamic stability at 300 K of MoS_2 monolayer, NO adsorbed MoS_2 (NO_MoS_2) and NO_2 adsorbed MoS_2 ($NO_2\_MoS_2$) are evaluated through ab initio molecular dynamics (AIMD) simulations. The figures present configurations after (a) 2.5 ps, (b) 5 ps, and (c) 7 ps.

References

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