Supporting Information

$MoTe_2$/InN van der Waals Heterostructures for Gas Sensors: A DFT Study

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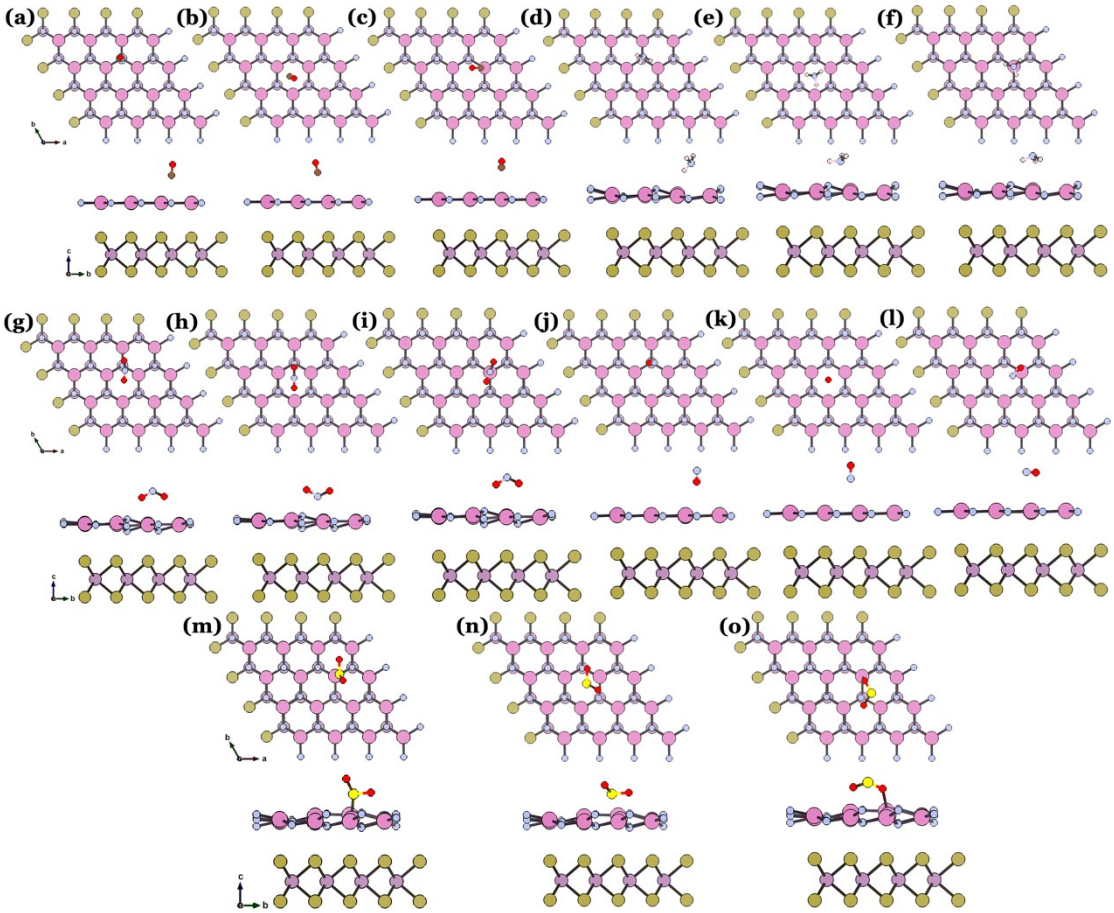

Figure S1. (Top/side view) Possible adsorption configurations of (a-c) CO, (d-f) NH_3, (g-i) NO_2, (j-l) NO, and (m-o) SO_2 gas molecules on top of the $MoTe_2$/InN vdW heterostructure. The possible adsorption sites are T_N, Hollow site, along with possible orientations on T_{In} (Atom colour code purple, Mo; light-brown, Te; pink, In; white, N)

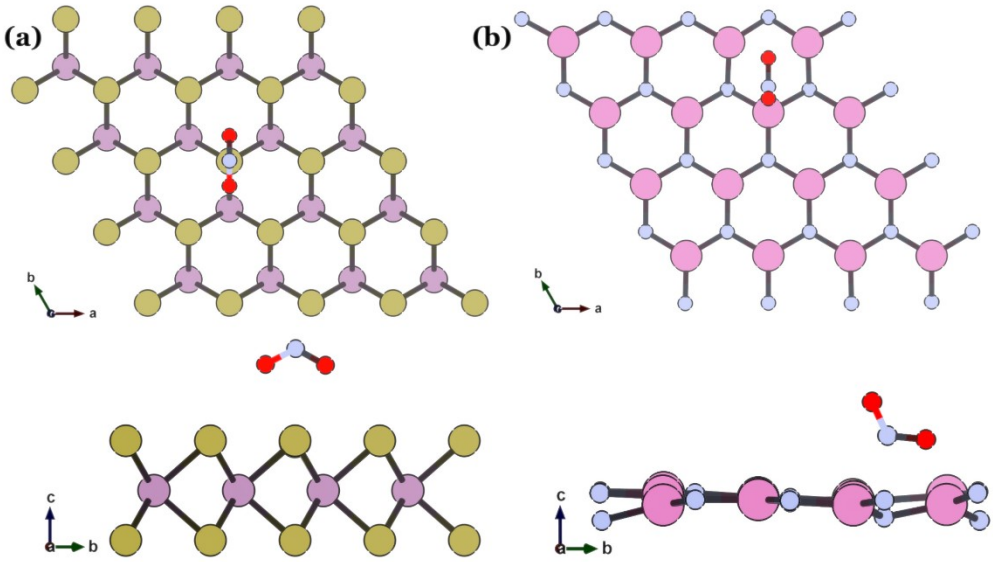

Figure S2. (Top/side view) The most energetically favourable adsorption configurations of NO_2 gas molecule on (a) $MoTe_2$ and (b) InN individual monolayer surfaces. (Atom colour code purple, Mo; light-brown, Te; pink, In; white, N; red, O)

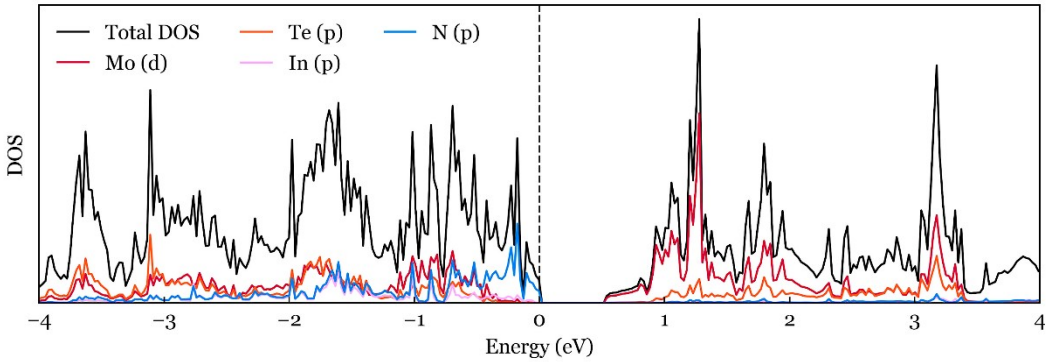

Figure S3. Total density of states (TDOS) and partial density of states (PDOS) for pristine $MoTe_2$/InN vdW heterostructure before the adsorption of gas molecules. (Note: Fermi level has been shifted to zero)

Table S1. Calculated adsorption energy (E_{ads}), the shortest distance between gas molecules and the adsorbent (d), and net Bader charge on the gas molecule (positive/negative sign of charge transfer denotes the transfer direction from/to the heterostructure).

Gas Molecule	Adsorption Site	E_{ads}(eV)	d(Å)	ΔQ(e)
CO	$T_{(N)}$	−0.21	2.90	+ 0.01
	$T_{(Hollow)}$	−0.18	3.02	+ 0.008
	Orientation	−0.13	3.19	+ 0.002
NH_3	$T_{(N)}$	−0.97	2.73	−0.078
	$T_{(Hollow)}$	−0.94	2.86	−0.069
	Orientation	−0.90	2.94	−0.061
NO_2	$T_{(N)}$	−0.51	3.41	+ 0.32
	$T_{(Hollow)}$	−0.84	2.42	+ 0.48
	Orientation	−0.55	3.30	+ 0.33
NO	$T_{(N)}$	−0.21	3.14	+ 0.07
	$T_{(Hollow)}$	−0.19	3.12	+ 0.068
	Orientation	−0.16	3.31	+ 0.063
SO_2	$T_{(In)}$	−2.09	2.25	+ 0.21
	$T_{(Hollow)}$	−0.93	2.65	+ 0.13
	Orientation	−0.24	3.32	+ 0.07

Table S2. Favourable adsorption site, calculated adsorption energy (E_{ads}), the shortest distance between NO_2 and the adsorbent (d), net Bader charge on the NO_2 gas molecule (positive/negative sign of charge transfer denotes the transfer direction from/to the monolayer), and the magnetic moment upon adsorption of NO_2 on individual $MoTe_2$ and InN monolayers.

Substrate	Adsorption site	E_{ads} (eV)	d (Å)	ΔQ (e)	Magnetic moment (μB)
$MoTe_2$	T_{Te}	−0.39	2.79	+ 0.32	+ 0.9999
InN	T_{In}	−0.55	2.2	−0.62	−0.9999

Table S3. The band gap (E_g), and effective masses of electron (m^*_e) and hole carriers (m^*_h) of

Gas molecule	E_g (eV)	$m^*_e(m_0)$		$m^*_h(m_0)$			
		K—M (Γ)	[Γ,M]—M	K—M (Γ)	Γ—M (K)	[M,K] —M	[k, Γ] — Γ
Pristine	0.52	0.43 (0.42)	—	1.41 (1.36)	—	—	—
CO	0.67	0.43 (0.42)	—	1.52 (1.39)	—	—	—
NH_3	0.97	0.45 (0.44)	—	—	2.31 (2.10)	—	—
NO_2	0.87	0.44 (0.43)	—	—	—	—	9.52
NO	0.78	—	0.43	—	—	1.77	—
SO_2	0.99	0.47 (0.45)	—	—	1.19 (1.52)	—	—

$MoTe_2$/InN vdW heterostructure with various adsorbed gas molecules.

Appendix A. Representative VASP INCAR file (geometrical relaxation of NO_2 on the surface of $MoTe_2$/InN vdW heterostructure, 4 × 4 unit cell)

Global Parameters
SYSTEM = MoTe2InN_NO2_4x4x1 (Title string)
ISTART = 0 (Starting job, begin from scratch)
ICHARG = 2 (Take superposition of initial atomic charge densities)
ISPIN. = 2 (Spin polarized DFT)
LREAL = .F. (Projection is done in reciprocal space)
PREC = Accurate (Precision level)
LWAVE = .T. (Write WAVECAR to the file)
LCHARG = .T. (Write CHGCAR to the file)
ADDGRID = .T. (Increase grid to help GGA convergence)

Electronic Relaxation
NELM = 100 (Max number of electronic SCF steps)
EDIFF = 1E-4 (SCF energy convergence in eV)
ENCUT = 450 (cut-off energy of plane wave basis set in eV)
ALGO = Fast (robust mixture of the Davidson and RMM-DIIS algorithms)
ISMEAR = 0 (Gaussian smearing)
SIGMA = 0.2 (width of the smearing in eV)

Ionic Relaxation
NSW = 300 (Max ionic steps or iterations)
EDIFFG = -0.01 (Ionic convergence eV/AA)
IBRION = 2 (Ionic relaxation conjugate gradient algorithm)
ISIF = 4 (lattice/atomic coordinates relaxation, fixed volume)
ISYM = 2 (Memory conserving symmetrization of the charge density)
POTIM = 0.5

vdW Corrections
GGA = OR (optPBE exchange & PBE correlation)
LUSE_VDW = .T. (switches on the use of a nonlocal vdW-DF functional)
AGGAC = 0.0
LASPH = .T. (non-spherical contributions from the gradient corrections)