Supplementary Information

Tailoring Janus In_2SeTe Monolayers with Al Doping: A Computational Study for NO_x Sensing Applications

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Table S I The lattice constant a; bond lengths of In-In (d1,d4), In-Se(d2,d5) and In-Te (d3,d6); bond angles of In-In-Se (θ1), In-In-Te (θ2), In-Se-In(θ3) and In-Te-In (θ4); the thickness layer(t); the band gap (E_g); VBM/CBM positions.

Type of Material	**a(Å)**	**d1(Å) d2(Å) d3(Å)**	**t(Å)**	**θ1(°) θ2(°) θ3(°) θ4(°)**	**E_g(eV)**	**Stability**	**VBM/CBM positions**
In_2SeTe	4.038	2.768, 2.684, 2.815	5.4	117.938°, 118.175°, 98.630°, 92.546°	1.192	Dynamically Stable	Γ- Γ
Al-Doped In_2SeTe	**a(Å)**	**d4(Å) d5(Å) d6(Å)**	**t(Å)**	**θ5(°) θ6(°) θ7(°) θ8(°)**	**E_g(eV)**	**Stability**	**VBM/CBM positions**
	4.054	2.767, 2.712, 2.809	5.34	116.296°, 122.713°, 98.540°, 95.217°	1.109	Dynamically Stable	Γ- Γ

Table S II Comparison of lattice constant, thickness, In-Se and In-Te bond lengths, and band gap(PBE) of Pristine In_2SeTe and Al-Doped In_2SeTe with other theoretical studies of In_2SeTe

Reference / System	**Lattice constant *a* (Å)**	**Thickness *l* (Å)**	**In–Se bond length d_1 (Å)**	**In–In bond length d_1 (Å)**	**In–Te bond length d_2 (Å)**	**Bond angle In-In-Se (θ1)**	**Bond angle In-In-Te (θ1)**	**Band gap PBE (eV)**
This work (pristine In_2SeTe)	**4.038**	**5.4**	**2.684**	**2.768**	**2.815**	**117.938**	**122.797**	**1.192**
This work (Al-doped In_2SeTe)	**4.054**	**5.3**	**2.712**	**2.767**	**2.809**	**116.296**	**122.713**	**1.109**
In_2SeTe [31]	**4.234**	**5.466**	**2.709**	**2.827**	**2.854**	**115.509**	**121.070**	**1.075**
In_2SeTe [30]	**4.23**	**6.02**	**—**	**2.83**	**—**	**—**	**—**	**1.38**
In_2SeTe [29]	**4.238**	**5.532**	**2.731**	**2.838**	**2.861**	**—**	**—**	**1.137**
In_2SeTe [18]	**4.18**	**5.55**	**2.71**	**2.82**	**2.84**	**—**	**—**	**1.07**

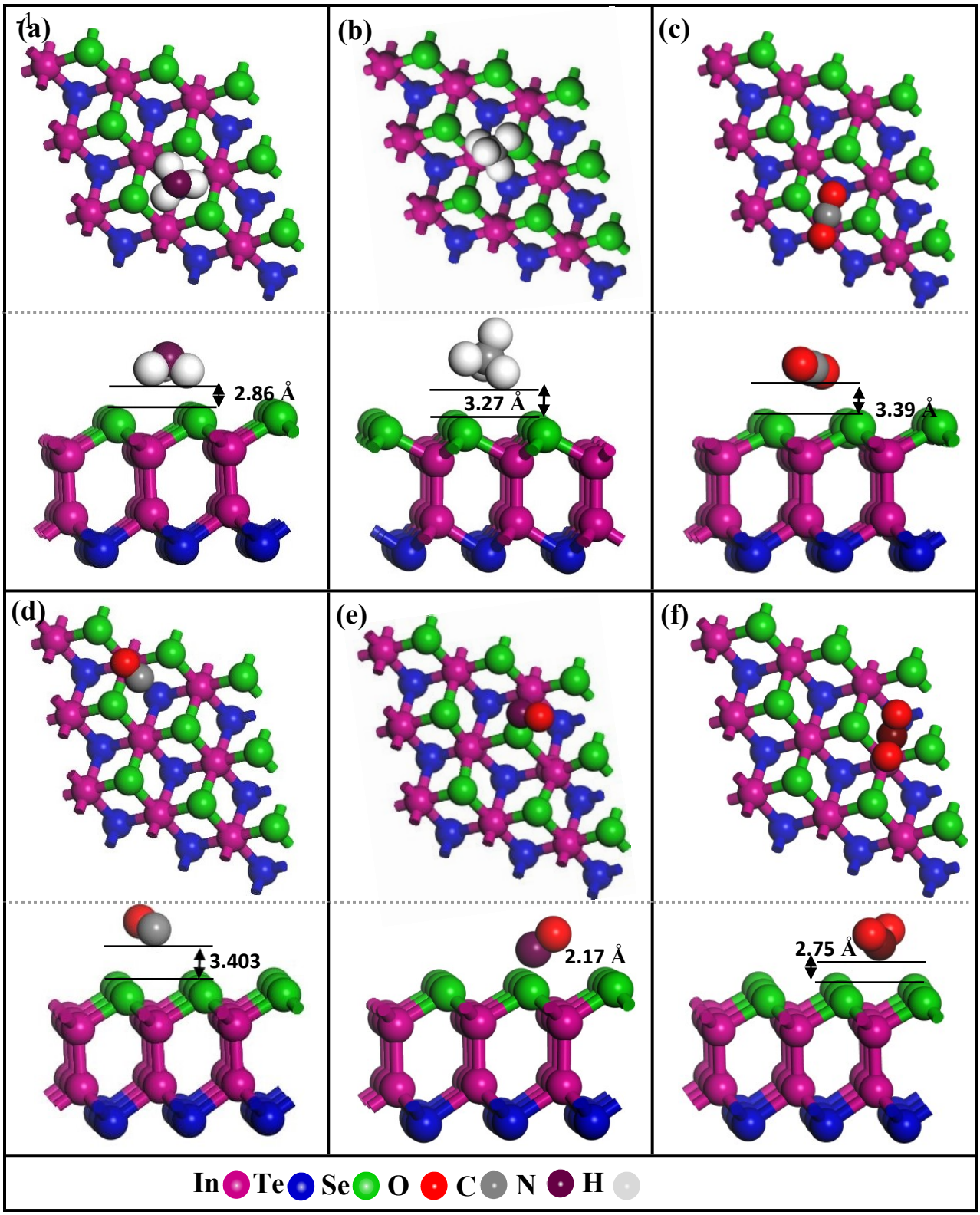

Fig. S1 Top View and Side View of In_2SeTe Monolayer after (a) NH_3 (b) CH_4, (c) CO_2, (d) CO, (e) NO and (f) NO_2 gas adsorption.

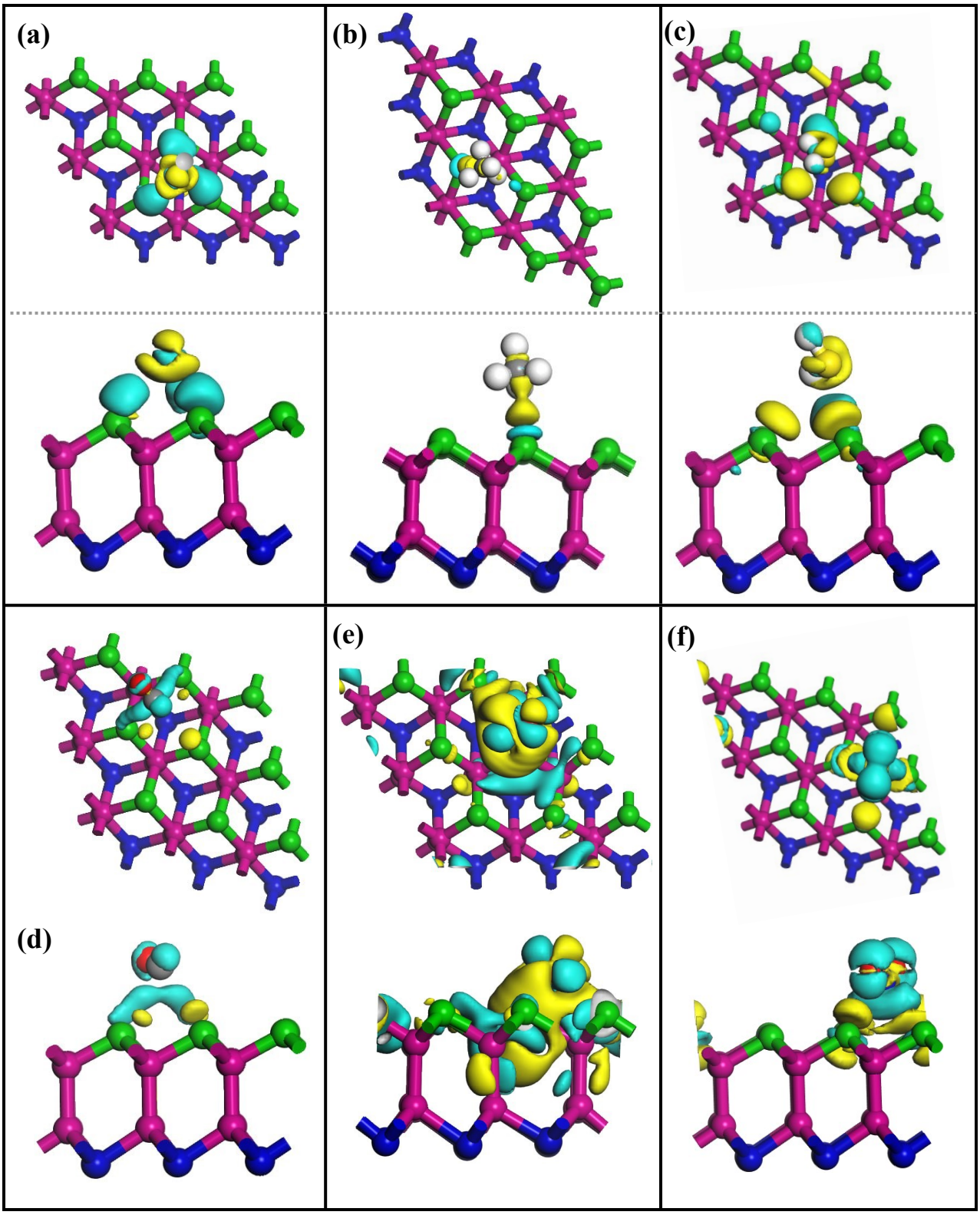
(a)
(b)
(c)
(d)
(e)
(f)

Fig. S2 Top View and Side View of Charge Density of In_2SeTe Monolayer after (a) NH_3 (b) CH_4, (c) CO_2, (d) CO, (e) NO and (f) NO_2 gas adsorption.

Table S III Variation of Bandgap and Sensitivity with Doping Percentage

%Doping	Bandgap (Without gas Adsorption) (eV)	Bandgap		Change in Bandgap(ΔE_g)		Log_{10}(%Sensitivity)	
		After NO_2 Adsorption	After NO Adsorption	NO_2	NO	NO_2	NO
2.77%	**1.109**	**0.497**	**0.041**	**-0.612**	**-1.068**	**7.135**	**10.962**
5.5%	**0.965**	**0.282**	**0.054**	**-0.683**	**-0.911**	**7.731**	**9.645**
8.33%	**0.861**	**1.024**	**0.096**	**0.163**	**-0.765**	**1.98**	**8.420**
11.11%	**0.819**	**0.992**	**0.097**	**0.173**	**-0.722**	**1.99**	**8.059**

Table S IV (In-N/O) bond lengths for NO and NO_2 for Pristine and Al-doped In_2SeTe

Structure	Gas Molecules/Adsorption Configuration	Adsorption Height(h), Å	In-N/O
Pristine In_2SeTe	**NO_2**	2.75	3.377/3.253
	NO	2.17	3.018/3.082
Al-Doped In_2SeTe	**NO_2**	2.72	3.753/3.658
	NO	2.67	3.676/3.620

Table S V (In-Se/Te) bond lengths and bond distortion for NO and NO_2 for Pristine and Al-Doped In_2SeTe

Structure/Gas Molecules	NH_3	CH_4	CO	CO_2	NO	NO_2
Pristine In_2SeTe	2.678/2.807	2.643/2.800	2.683/2.816	2.679/2.805	2.681/2.812	2.672/2.824
Al-Doped In_2SeTe	2.709/2.799	2.709/2.799	2.716/2.799	2.709/2.799	2.709/2.812	2.716/2.809

Bond Distortion	0.031/0.008	0.066/0.001	0,033/0.017	0.030/0.006	0.028/0	0.044/0.015

Table S VI Sensitivity of different gas molecules adsorbed on pristine and Al-doped In_2SeTe monolayer, respectively

Gas Molecule	**Pristine In_2SeTe**		**Al-doped In_2SeTe**	
	Sensitivity (%)	**Log_{10}(Sensitivity%)**	**Sensitivity (%)**	**Log_{10}(Sensitivity%)**
NH_3	18.995	1.278	28.55	1.4556
CH_4	59.005	1.7708	10.14	1.0060
CO_2	3.4278	0.5350	7.43	0.8709
CO	5.6322	0.7506	12.29	1.0895
NO	7.249958×10^5	5.8603	9.17×10^{10}	10.9623
NO_2	2.653623×10^5	3.4238	1.367×10^7	7.1357

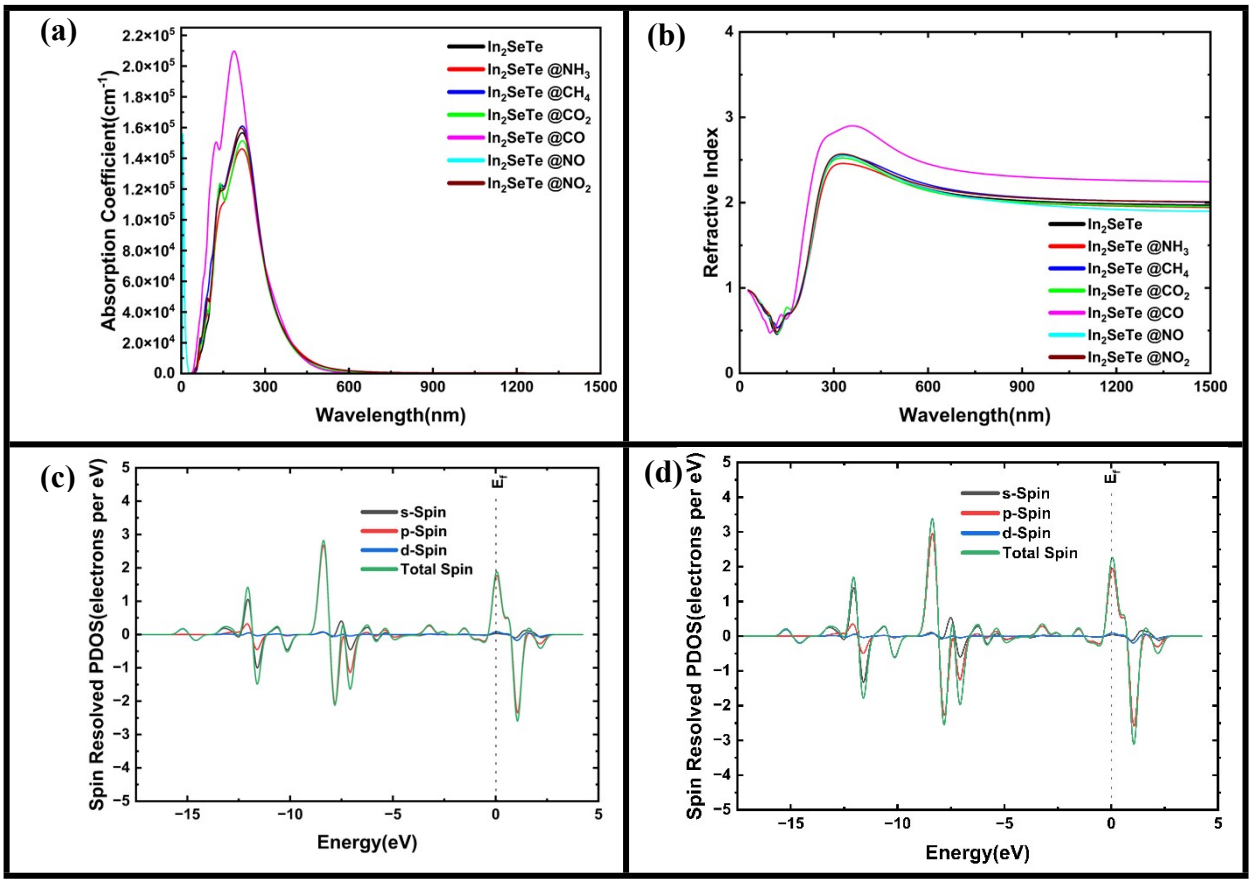

Fig. S3 (a) Absorption Coefficient, (b) Refractive Index of pristine In_2SeTe Monolayer, Spin Resolved PDOS of pristine In_2SeTe Monolayer for (c) NO, (d) NO_2