Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Supporting Information

Reversible Gas Capture by Ferroelectric Switch and 2D Molecule Multiferroics in In_2Se_3 Monolayer

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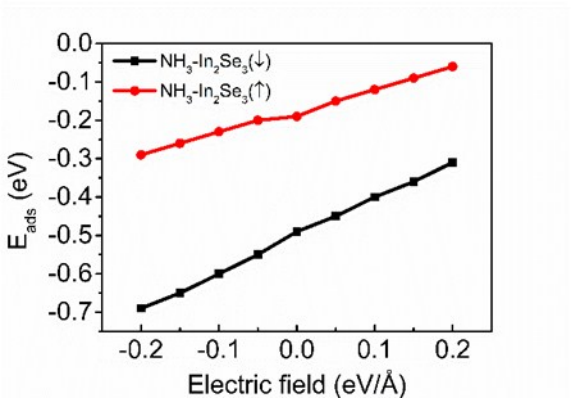

Fig. S1 Adsorption energy of NH_3 adsorbed on In_2Se_3 surfaces under different electric field.

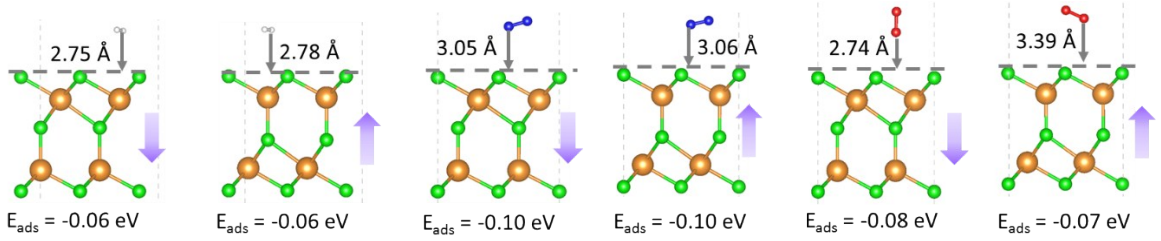

Fig. S2 The most stable configurations of H_2, O_2, N_2 onto P ↓ and P ↑ sides of In_2Se_3 monolayer. Corresponding adsorption distance and adsorption energy were also shown.

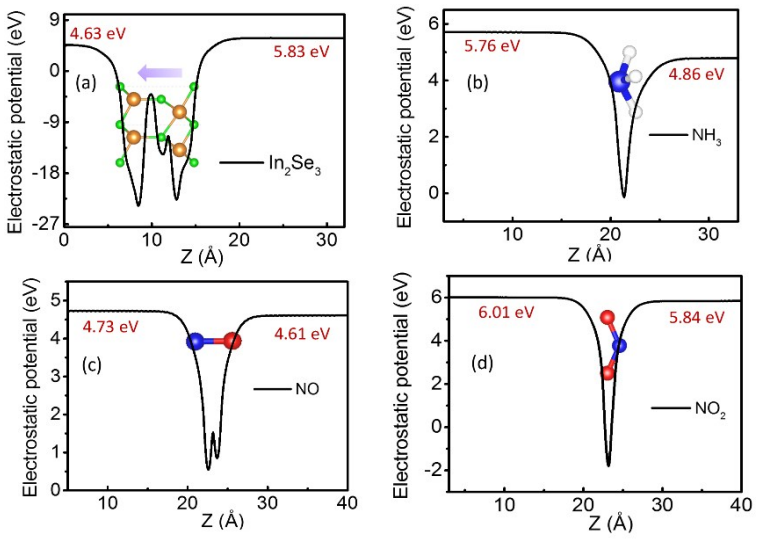

Fig. S3 Electrostatic potential of (a) pure In_2Se_3, (b) NH_3, (c) NO and (d) NO_2. Green, orange, white, blue and red balls present the Se, In, H, N and O atoms, respectively. The arrow represents the direction of electric polarization.

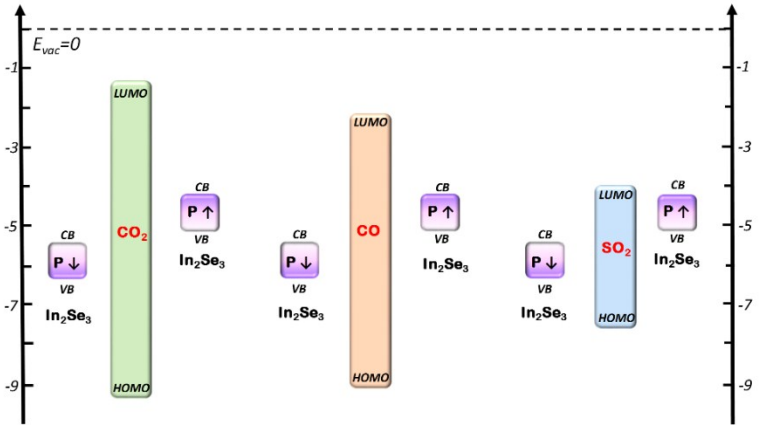

Fig. S4 Energy-level with respect to the vacuum level for In_2Se_3 (P ↓), In_2Se_3 (P ↑), CO_2, CO and SO_2.

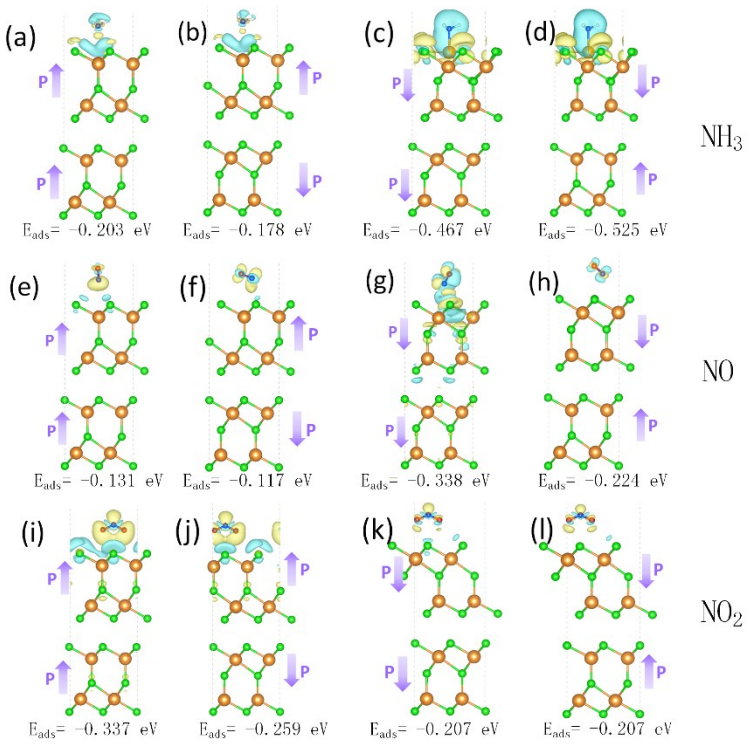

Fig. S5 Charge density difference and adsorption energies for NH_3 (a-d), NO (e-h) and NO_2 (i-l) on In_2Se_3 (P↑ ↑), In_2Se_3 (P↑ ↓), In_2Se_3 (P↓ ↓) and In_2Se_3 (P↓ ↑) surfaces, respectively. The yellow (cyan) region represents charge accumulation (depletion) and the isosurface value is 0.0004 e Å^{-3}. The purple arrow represents the direction of polarization. Green, orange, white, blue and red balls present the Se, In, H, N and O atoms, respectively. E_{ads} =E_{total}-E_{gas}-$E_{In2Se3\text{-}bilayer}$, where E_{total}, E_{gas} and $E_{In2Se3\text{-}bilayer}$ are energies of bilayer In_2Se_3 with adsorbed gas molecule, isolated gas molecule and pure In_2Se_3 bilayer.

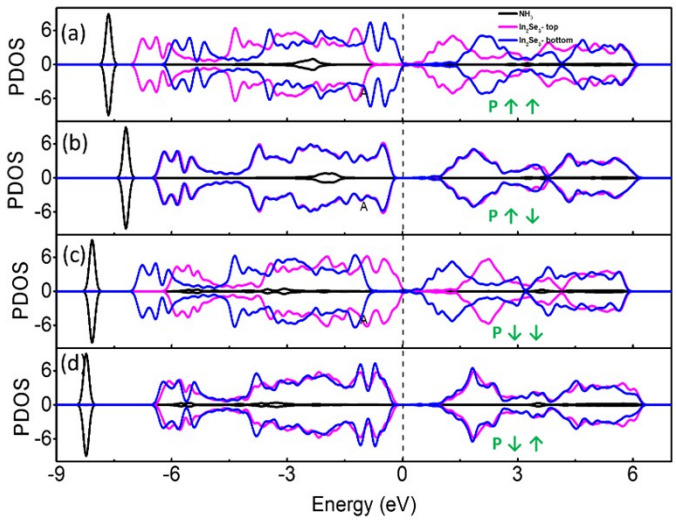

Fig. S6 Calculated projected density of states (PDOS) of NH_3 adsorption on (a) In_2Se_3 (P↑ ↑) (b) In_2Se_3 (P↑↓) (c) In_2Se_3 (P↓↓) and (d) In_2Se_3 (P↓↑) bilayer. Black, magenta and blue lines denote PDOS of NH_3, top layer In_2Se_3 and bottom layer In_2Se_3, respectively. The Fermi level is set to zero.

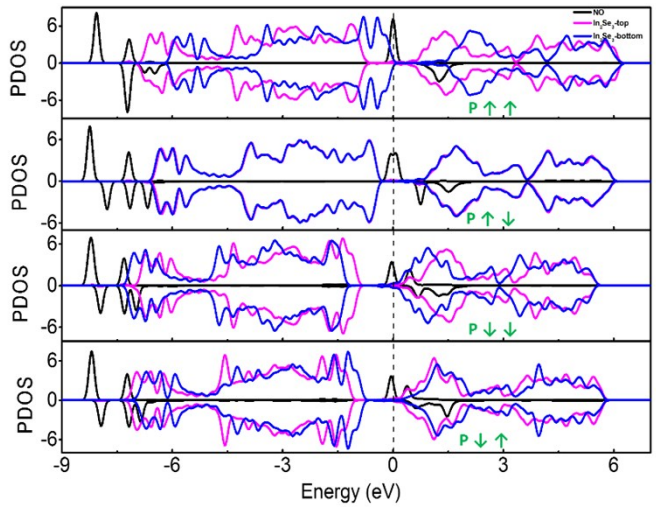

Fig. S7 Calculated projected density of states (PDOS) of NO adsorption on (a) In_2Se_3 (P↑↑) (b) In_2Se_3 (P↑↓) (c) In_2Se_3 (P↓↓) and (d) In_2Se_3 (P↓↑) bilayer. Black, magenta and blue lines denote PDOS of NO, top layer In_2Se_3 and bottom layer In_2Se_3, respectively. The Fermi level is set to zero.

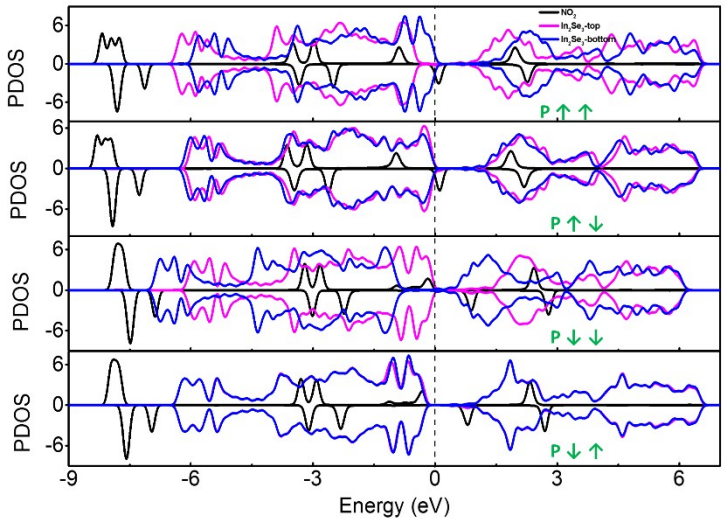

Fig. S8 Calculated projected density of states (PDOS) of NO_2 adsorption on (a) In_2Se_3 (P↑↑) (b) In_2Se_3 (P↑↓) (c) In_2Se_3 (P↓↓) and (d) In_2Se_3 (P↓↑) bilayer. Black, magenta and blue lines denote PDOS of NO_2, top layer In_2Se_3 and bottom layer In_2Se_3, respectively. The Fermi level is set to zero.

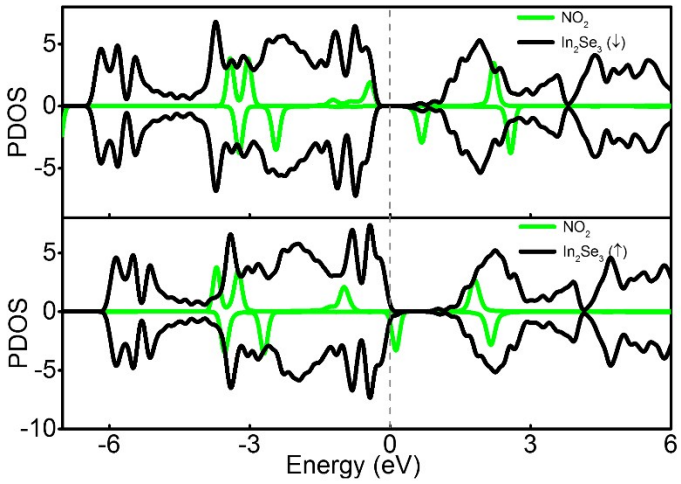

Fig. S9 Upper panel: PDOS for the NO_2 adsorbed In_2Se_3 (P ↓). Lower panel: PDOS for the NO_2 adsorbed In_2Se_3 (P ↑).

Table S1. The calculated magnetic moment of NO and NO_2 adsorbed In_2Se_3.

System	Magnetic Moment (μ_B)	System	Magnetic Moment (μ_B)
$NO+In_2Se_3$ (↓)	0.88	$NO_2+In_2Se_3$ (↓)	1.00
$NO+In_2Se_3$ (↑)	1.00	$NO_2+In_2Se_3$ (↑)	0.89
$NO+In_2Se_3$ (↑↑)	1.07	$NO_2+In_2Se_3$ (↑↑)	0.79
$NO+In_2Se_3$ (↑↓)	1.00	$NO_2+In_2Se_3$ (↑↓)	0.86
$NO+In_2Se_3$ (↓↑)	0.73	$NO_2+In_2Se_3$ (↓↑)	1.00
$NO+In_2Se_3$ (↓↓)	0.70	$NO_2+In_2Se_3$ (↓↓)	0.98

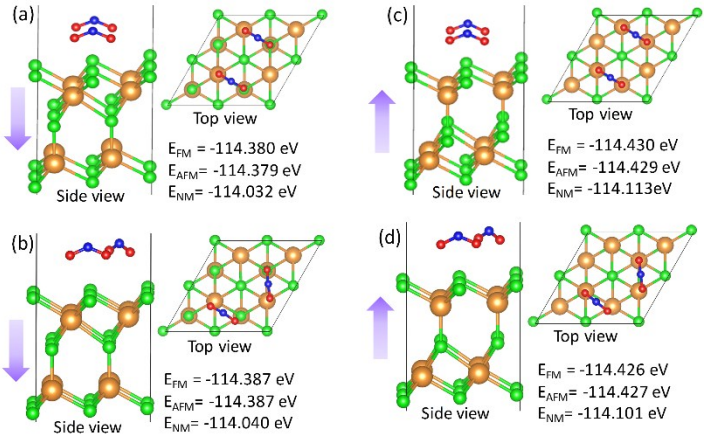

Fig. S10 (a-b) Geometric structures and energy of different magnetic coupling (ferromagnetic, antiferromagnetic and nonmagnetic coupling) between two NO_2 molecules on In_2Se_3 (P↓) surface and (c-d) In_2Se_3 (P↑) surface. The purple arrows indicate the directions of electric polarization. Green, orange, blue and red balls present the Se, In, N, and O atoms, respectively.

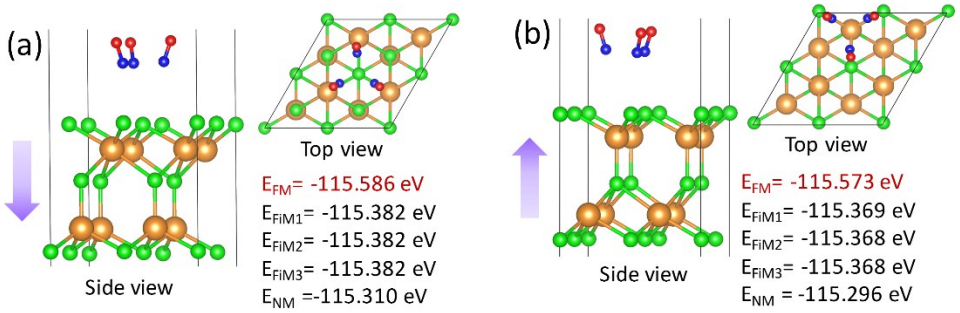

Fig. S11 (a-b) Geometric structures and energy of different magnetic coupling (ferromagnetic, ferrimagnetic and nonmagnetic coupling) between three NO molecules on In_2Se_3 (P↓) surface and In_2Se_3 (P↑) surface. The purple arrows indicate the directions of electric polarization. Green, orange, blue and red balls present the Se, In, N, and O atoms, respectively.