Ferroelectric In2Se3 Monolayer: A Promising Candidate as NH3 Gas Sensor and Capturer

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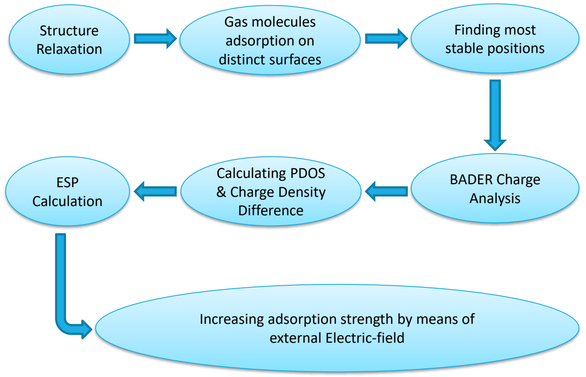
ABSTRACT

- 2D ferroelectrics present applications in wide range of electronics.
- Ferroelectric In_2Se_3 monolayer is a suitable candidate to be used as a gas sensor.
- in this work, different gas molecules adsorb on distinct surfaces of In_2Se_3 monolayer, and their adsorption behaviours are investigated.

OBJECTIVES



COMPUTATIONAL METHODS

- Density functional theory (DFT) calculations.
- The Vienna Ab initio Simulation Package (VASP) implementation[1].
- Perdew-Burke-Ernzerhof (PBE) version of the generalized gradient approximation (GGA) [2].
- Relaxing structures until the energy and force on each atom are less than 10^{-5} eV and 0.01 eV/Å, respectively.
- The Brillouin zone integration sampling by $6\times6\times1$ and $10\times10\times1$ *k*-grid mesh.
- a 2×2 supercell was used to simulate the periodic structure of In_2Se_3 monolayer.
- A vacuum space greater than 20 Å was applied in the *z* direction.
- $E_{ads} = E_{total} - E_{In2Se3} - E_{gas}$
- $\Delta\rho = \rho_{In2Se3+gas} - \rho_{In2Se3} - \rho_{gas}$

RESULTS

- **The lattice parameter is 4.06 Å and height of In_2Se_3 monolayer is 6.82 Å, which is consistent with other theorical studies.[3]**

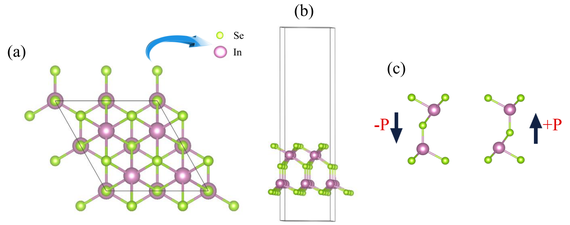


Figure 1: a schematic illustration of (a) top, and (b) side view of In_2Se_3 monolayer used for our calculations. (c) Two stable structures of In_2Se_3 which can be switch to each other by laterally moving the central Se atom and reorientation of top In atoms. Both surfaces have spontaneous electric polarization with opposite directions. Up and down arrows refer to positive and negative polarizations, respectively.

- **Adsorption energy and charge transfer for the most stable structures of CO, CO_2, H_2O, H_2S, NH_3, NO, NO_2, CH_4, and O_2 gas molecules are shown in Table 1.**
- **The obtained results are in complete agreement with previous study [4].**
- **There is different gas adsorption behaviours on distinct surfaces of In_2Se_3.**
- **In_2Se_3 is most preferred for NH_3 molecule with suitable adsorption strength and apparent charge transfer.**
- **NH_3 molecule is physically adsorbed on up-side, while its adsorption type is chemically for another side.**

Table 1: Adsorption energies, Charge transfers, and nearest distances between gas molecules and In_2Se_3 monolayer.

Gas	E_{ads} (eV)	CT (e)	$D_{gas\text{-}substrate}$ (Å)
NH_3 (up, down)	−0.15, −0.47	−0.0006, 0.1201	2.51, 2.27
CO (up, down)	−0.09, −0.09	−0.0142, −0.0153	3.5, 3.43
NO_2 (up, down)	−0.28, −0.3	−0.1852, −0.1530	2.78, 2.56
CO_2 (up, down)	−0.13, −0.13	−0.0233, −0.0213	3.4, 3.37
H_2O (up, down)	−0.12, −0.16	−0.0269, −0.0283	2.55, 2.28
H_2S (up, down)	−0.12, −0.12	−0.008, −0.007	2.99, 2.96
NO (up, down)	−0.1, −0.35	−0.0058, −0.0359	3.1, 2.43
O_2 (up, down)	−0.12, −0.25	−0.1059, −0.2169	3.24, 1.74
CH_4 (up, down)	−0.12, −0.13	0.9665, 0.9428	2.74, 2.75
H_2 (up, down)	−0.05, −0.05	−0.0189, −0.0059	2.77, 2.92

- **There is noticeable structure deformation for NH_3 adsorption on down-side and the N atom of gas molecule is bonded with In atom of substrate in the second layer.**
- **For another side, the structure of substrate is not strongly distorted and there is no chemical bonding between gas molecule and the substrate.**

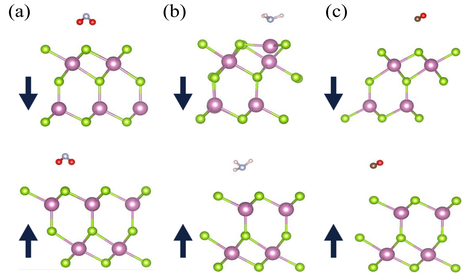


Figure 2: Most stable structure for the adsorption of various gas molecules on different surfaces of In_2Se_3: (a) NO_2, (b) NH_3, and (c) CO adsorption.

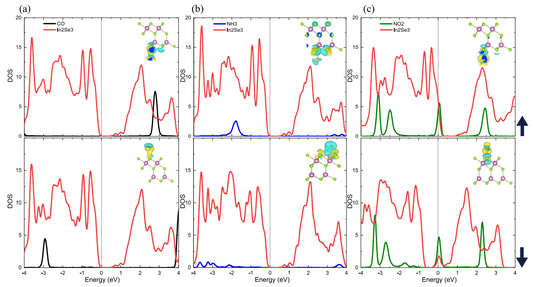


Figure 3: The PDOS of (a) CO, (b) NH_3, and (c) NO_2 molecules adsorbed on In_2Se_3 monolayer for up and down sides.

- **The controllable adsorption manner for different gas molecules is obtained using an external Electric-field.**

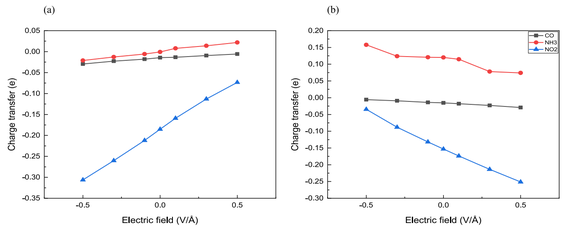


Figure 4: Electric field effects on charge transfer of CO, NH_3, and NO_2 molecules adsorbed on (a) up and (b) down sides of In_2Se_3 monolayer.

- **Different DOS, CDD, and ESP for adsorption on distinct surfaces of the substrate, demonstrate the accuracy of research findings.**

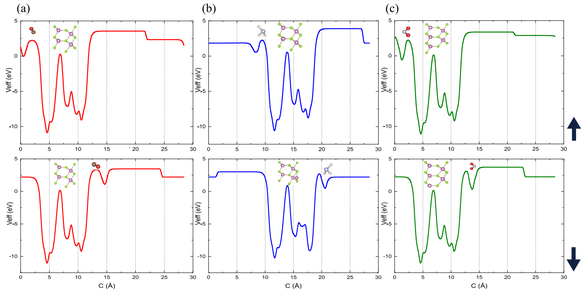


Figure 5: Electrostatic surface potential (ESP) for (a) CO, (b) NH_3, and (c) NO_2 gas molecule adsorption on up and down sides of In_2Se_3 monolayer.

CONCLUSIONS

- **Based on first principles calculations, we found that In_2Se_3 monolayer is a suitable substrate for NH_3 gas capture with appropriate adsorption energy.**
- **There is different adsorption energy on different surfaces of In_2Se_3, so an acceptable approach to capture or release NO, NO_2, NH_3, and O_2 gas molecules has been earned.**
- **The effect of external electric-filed on adsorption strength of NO_2, NH_3, and CO molecules, represents an effective way for achieving reversible gas capture.**

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CONTACT

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