First principle investigation of pyridinic N-doped graphene as a Potential SO_2 gas sensor

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Pyridinic N-doped graphene (PNG) is of great importance in gas-sensing devices due to doping and defects that create an active region on the surface through overlapping charge and spin densities. Sulfur dioxide (SO_2), a harmful and toxic pollutant, combines with nitrogen oxides leading to acid rain and damaging ecological balance. Herein, we explore the SO_2 sensing potential of pyridinic N-doped graphene (PNG) under the framework of spin-polarized density functional theory incorporating Van der Waals correction and ab initio molecular dynamics (AIMD) simulation in detail. Our findings imply that SO_2 binds with energies between -0.30 to -0.80 eV, which shows that the PNG monolayer towards SO_2 detection is reversible. The environmental selectivity of pyridinic N-doped graphene towards SO_2 was also revealed by studying the effect of major environmental composites such as CO_2, N_2, O_2, and H_2O. Furthermore, the adsorption potential of SO_2 on PNG can be strengthened or weakened by applying external strains or electric fields, which is highly desirable to control the sensing performance of the monolayers. Our work is a step toward the vision of developing efficient gas sensors for the detection of toxic-gas molecules in the environment.

References

[1] Nath, U., Sarma, M., J. Phys. Chem. A 127(5), (2023) 1112-1123.

Figures

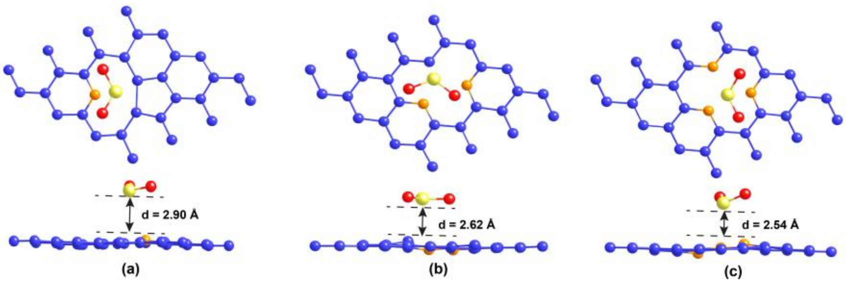

Figure 1: Optimized structures of the preferred adsorption configuration of SO_2 molecules on (a) pysvn1, (b) pysvn2, and (c) pysvn3.

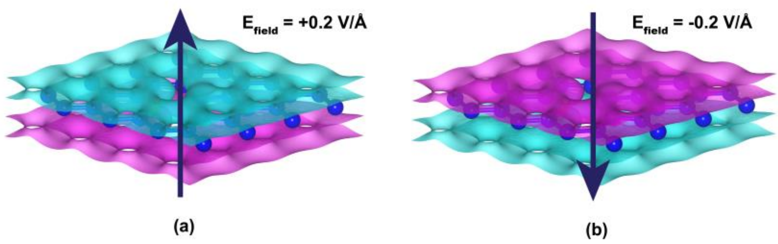

Figure 2: Charge density difference (CDD) of the pysvn1 monolayer by (a) positive and (b) negative electric fields. Charge accumulation and depletion are shown in purple and cyan iso-surfaces, respectively.