Interaction of gas molecules with a monoatomic MoS_2 layer

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Abstract

The potential applications of monolayer MoS_2 as a chemical gas sensor are explored in the present work by means of Density Functional Theory (DFT) simulations. Graphene has been proposed as the ultimate material for sensor applications, but it lacks selectivity in the recognition of different chemical species. Monolayer MoS_2, in contrast, has been shown to be much more selective, and it is hence a good alternative to graphene as the active component of ultrascaled, 2D materials-based gas sensors.

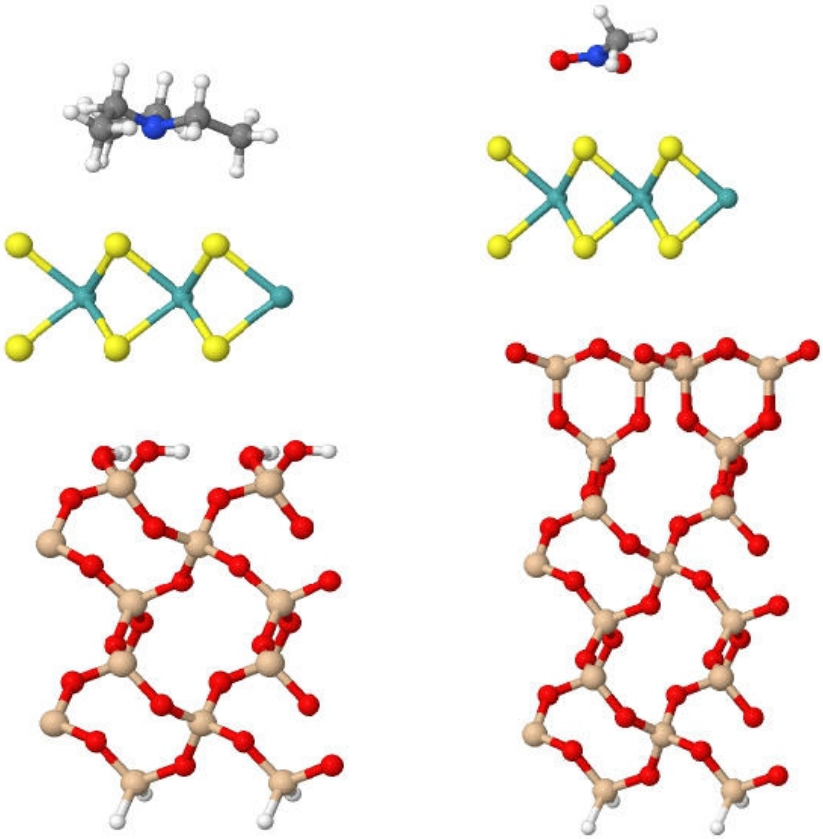
Motivated by the work of Perkins *et al*. [1], we study the chemical reactivity of single-layer MoS_2 by means of DFT simulations. We have chosen two molecules with dissimilar chemical behavior, namely triethylamine, which typically behaves as an electron donor, and nitromethane, which tends to act as an electron acceptor. Both molecules have been experimentally proven to react in very different ways to the monolayer MoS_2-based sensor.

After the characterization of the Potential Energy Surface (PES) for both molecules on the monolayer surface, we selected the most stable configurations and studied the influence of a SiO_2 substrate under the molecule-on-MoS_2 compounds, using two reconstructions of the SiO_2 surface to test the impact of different atomic rearrangements at the oxide/MoS_2 interface. The structural and electronic properties of such systems have been analysed and in the present work the results are contrasted against the experimental evidence.

References

[1] Perkins, F. K., Friedman, A. L., Cobas, E., Campbell, P. M., Jernigan, G. G., and Jonker, B. T., Nano Letters, **13** (2013), 668.

Figures



Left panel: a triethylamine (TEA) molecule on top of the MoS_2 monolayer on a silanol substrate
Right panel: a nitromethane (NM) molecule on top of the MoS_2 monolayer on a siloxane substrate