Sensing capabilities of a single-layer MoS_2 substrate for molecule detection

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Abstract

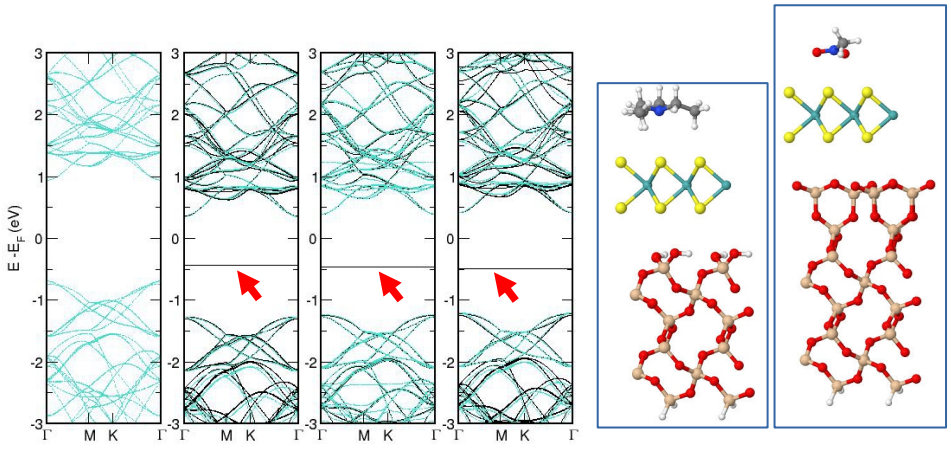
Motivated by the work of Perkins *et al*. [1], we investigated, by means of DFT simulations, the potential capabilities of a monolayer MoS_2 to detect different molecular species. Although graphene has been proposed as the ultimate material for sensor applications, it lacks selectivity in the recognition of different chemical species. In contrast, Perkins *et al*. showed that monolayer MoS_2 is capable to distinguish between molecules with different chemical character, hence being a good alternative to graphene as the active component of ultrascaled, 2D materials-based gas sensors.

Following the experiment by Perkins *et al*., the molecular species chosen for our study were triethylamine, which typically behaves as an electron donor, and nitromethane, which tends to act as an electron acceptor. After the characterization of the Potential Energy Surface (PES) for both molecules on the monolayer surface, we studied the influence of two possible reconstructions of a SiO_2 substrate under the molecule-on-MoS_2 compounds, using both the silanol and the siloxane reconstructions 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. The study has been extended to the interaction of the MoS_2 monolayer with acetates and triflates of transition metals of the fourth period.

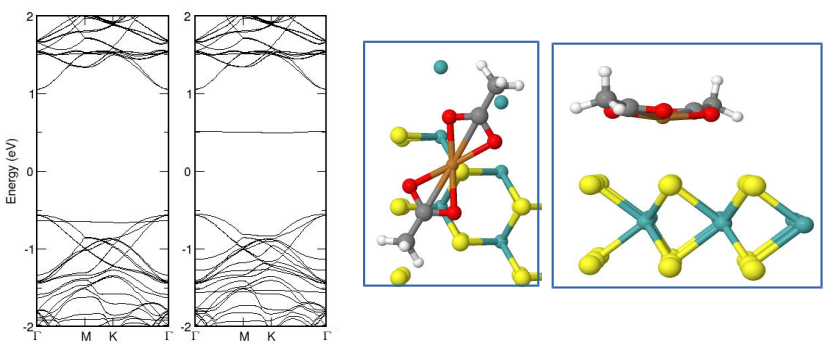
References

[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: Bandstructure of the 3x3 MoS_2 supercell, the TEA/MoS_2, the TEA/MoS_2/silanol and the NM/MoS_2/siloxane
Center 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



Left panel: Bandstructures for the spin up (left) and down (right) states of the copper(II) acetate ($Cu(OAc)_2$) on top of the 3x3 MoS_2 supercell
Center and right panels: top and side view of the $Cu(OAc)_2$ molecule on top of the MoS_2 monolayer