The effect of adsorption of gas molecules on electronic and transport properties of nanostructures graphene membrane.

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Abstract
The unique electronic structure and physical properties of graphene make it very sensitive to external influences. In particular, gas molecules adsorbed on its 2D nanostructured surface can significantly affect the electronic structure and transport properties of graphene sheets. It was shown in literature [1] that this effect could be potentially used for development of highly efficient gas sensor devices. However such development requires the knowing of fundamental processes which happens in the nanostructured graphene. In that work we present the extended study of the effect of physisorbed gas molecules on electronic and transport properties of nanostructures graphene membranes. In opposite to many other works (e.g. [2]) we use to study the collective effect of adsorbed molecules on conductance and transmission spectra's. That allows us to avoid many difficulties related to precise positioning of molecules relative to defects. The subsequent Car-Parinello molecular dynamics shows that the calculated favorite geometries allow to represent accurately the averaged distribution of gas molecules on defects. The balance of adsorption/clustering is also discussed.
The results could be interesting for researchers working on the development of the real prototype of gas sensor devices.

References

[1]. J. K. Holt, H. G. Park et al., Science **312**(2006)**,** 1034
[2] B. Huang, Z. Li, Park et al., J. Phys. Chem. C, **112**(2008), 13442

Figures

Fig. 1. The studied nanostructured defects on PBS graphene surface with carbone monoxide molecules physisorbed on it.

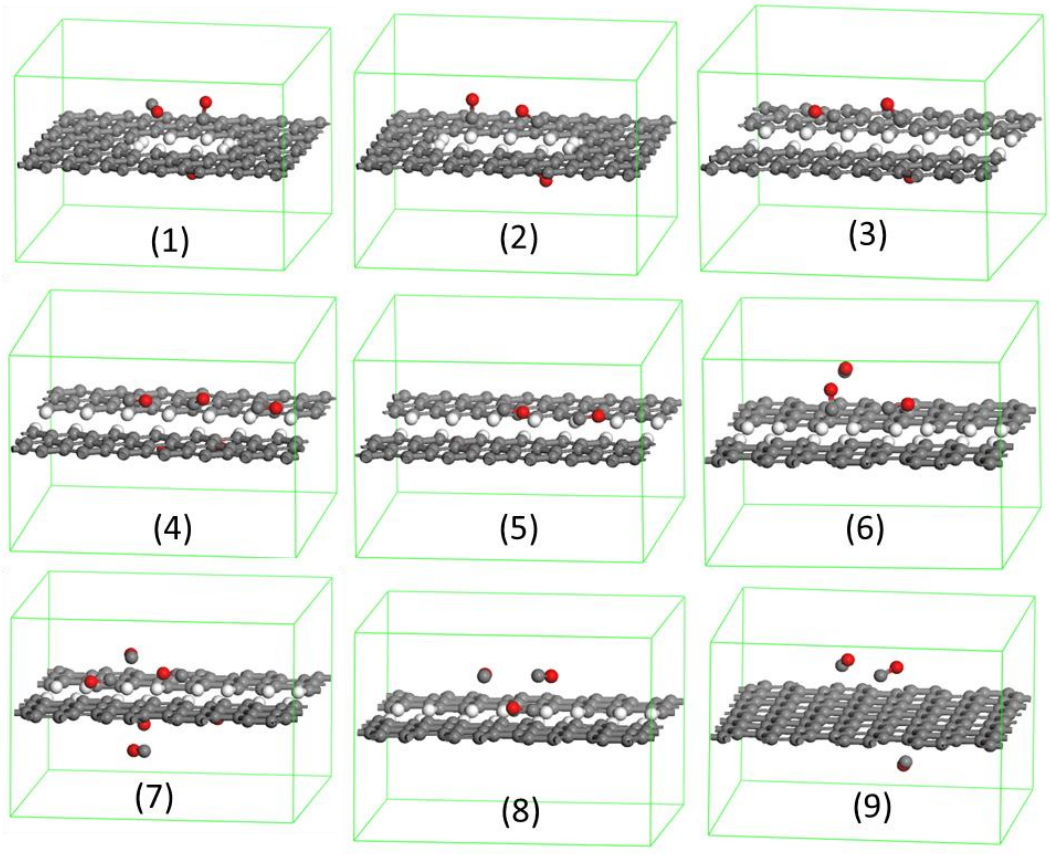

Fig. 2. Adsorption energies (CO, H_2O, H_2S and NH_3 molecules) calculated by PBC-DFT approach for the different types of defects.

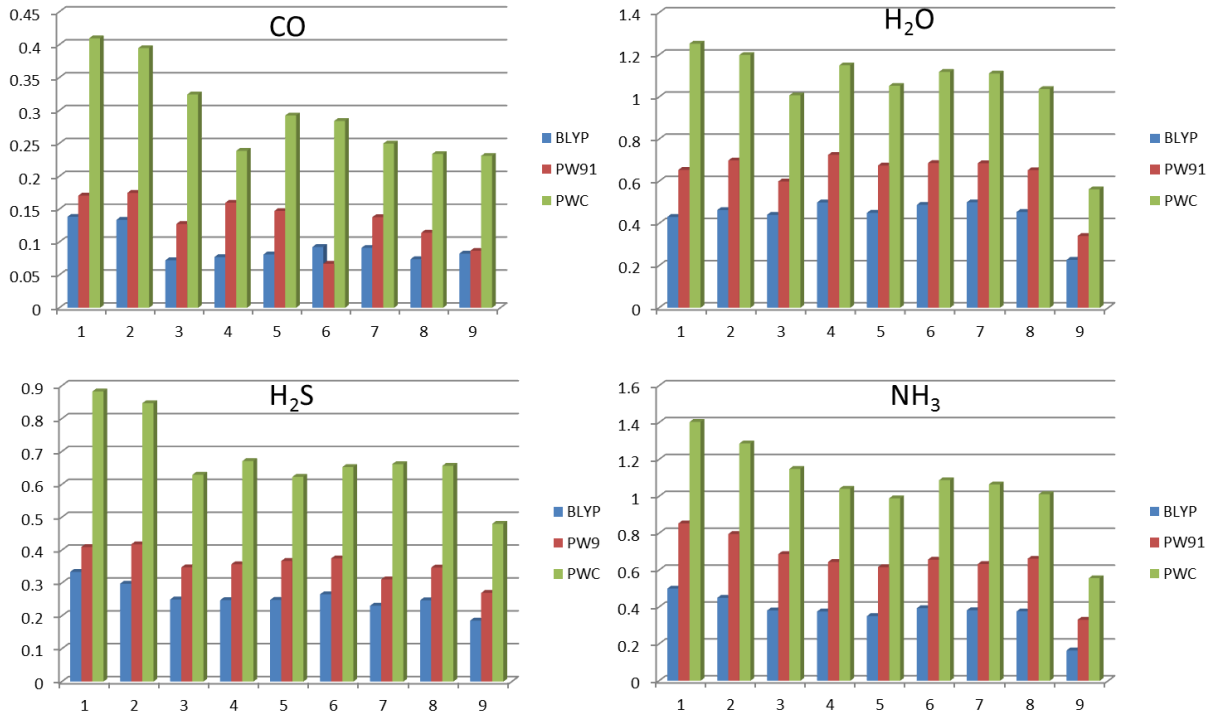

Fig. 3. The effect of adsorption of CO and H2O molecules on DFT gap (blue - BLYP, red - PW91, green PWC - functionals) for two types of defects compare to the plane graphene surface