# Structural and electronic properties of molecules adsorption on Blue Phosphorene

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Since the discovery of the two-dimensional (2D) materials such as Graphene, silicene, germanene, etc., with unique optical, electrical, mechanical, transport and gas sensing properties, the interest in the study of these 2D systems has increased significantly. Searching for new alternatives of gas sensing devices, it has been found that one of the most stable allotrope of phosphorus, the black phosphorous or phosphorene, is a good candidate for such applications. Phosphorene is a direct gap semiconductor with an energy gap of the order between 1 and 2 eV, high carrier mobility and armchair ridges [1]. Because of black phosphorene discovery the interest in the study of different allotropes of phosphorus has attracted the attention of the researchers. In addition to black phosphorene, it has been predicted the existence of a second allotrope, the blue phosphorene, which is an indirect gap semiconductor with a gap of the order of 2 eV. This 2D material displays high carrier mobility similar to that of black phosphorus, it has a buckled honeycomb lattice with zigzag ridges [2]. It is important to study blue phosphorene because it displays different electronic, sensing and transport properties in comparison with its counterpart, the black phosphorene.

In this work, the density functional theory (DFT) is applied as implemented in the computational code SIESTA, to investigate molecules adsorption on pristine, Al- doped and a single vacancy blue phosphorene. Five molecules are considered to explore the efficiency and versatility of the blue phosphorene. We want to show that blue phosphorene may be a possible solution of different current problems, such as the environmental pollution and the lack of control getting sub-products in chemical processes that affect the human health. Results show that Al-doped blue phosphorene have stronger interaction energy than pristine and single vacancy blue phosphorene. Single vacancy blue phosphorene has the weakest interaction energy, however it displays magnetic properties. On the other hand, pristine blue phosphorene faces physisorption with no magnetic properties.

## References

[1] H. Liu, A. T. Neal, Z. Zhu, Z. Luo, X. Xu, D. Tománek, P. D. Ye, Phosphorene: An Unexplored 2D Semiconductor with a High Hole Mobility, 8, 4, 4033-4041 (2015).
[2] Z. Zhu and D. Tománek, Semiconducting Layered Blue Phosphorus: A Computational Study, Physical Review Letters, 112, 176802 (2014).