# ADSORPTION OF ATOMS AND MOLECULES ON GRAPHENE-LIKE AND BOROPHENE MONOLAYERS: ISSUES OF CONCERN AND SOURCES OF ERROR

**A. Postnikov and K. Zhour**
*LCP-A2MC, Université de Lorraine, Metz, France*

Modern first-principles schemes, if correctly used with a careful choice of corresponding technical cutoffs, are supposed to yield practically identical results [1]. However, different routine calculations of as "conventional" properties as e.g. adsorption energies, for a system on which no established benchmarks are known, yield results which may be quite at variance. We overview a series of our recent calculations of adsorption energies for (alkali metal) atoms and small molecules on hexagonal $BC_3$ monolayer, of molecules on $NC_6B$-2 monolayer, and molecules on *Pmmn*8-borophene. Some of these results are novel (predictive) whereas the others follow a tradition of earlier studies. The results concerning alkali metal atoms on $BC_3$ are recently published in [2]. The calculation methods used, – Quantum Espresso [3], Siesta [4] and VASP [5], – were in some cases applied for the same task, for test purposes, but more typically exploited in the field of relative strength of one or the other code, aimed at different trial situations.

Offering here only a brief discussion of "chemical" (materials-science) component of the results, we turn to analysing the reasons why the findings reported by different groups can be so different. Possible sources of error are basis set superposition, neglected magnetic moment (e.g., of an alcali metal atom), insufficient supercell size, algorithms for calculating adsorption energy which do not sufficiently compensate systematic errors. A careful analysis of results of different methods in comparison, checking the convergence of sensitive cutoffs, an inspection of "smooth" trends (e.g., interaction energy as function of distance), rather than of singular energy difference etc. assigns certain credibility to our findings.

## References

[1] Lejaeghere K *et al.* : Reproducibility in density functional theory calculations of solids. Science. 2018; 351(6280): aad3000.

[2] Zhour K and Postnikov A: Theoretical Mapping of Interaction between Alkali Metal Atoms Adsorbed on Graphene-Like $BC_3$ Monolayer. Phys.Stat.Sol.(b). 2021; https://doi.org/10.1002/pssb.202100131.

[3] Giannozzi P *et al.*: QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. J. Phys. Condens. Matter. 2009; 21(39): 395502. Advanced capabilities for materials modelling with QUANTUM ESPRESSO. J. Phys. Condens. Matter. 2017; 29(46): 465901.

[4] García A *et al.*: SIESTA: Recent developments and applications. J.Chem.Phys. 2020; 152: 204108.

[5] Kresse G and Hafner J. *Ab initio* molecular dynamics for liquid metals. 1993, Phys.Rev. B. 47: 558. *Ab initio* molecular-dynamics simulation of the liquid-metal–amorphous-semiconductor transition in germanium. 1994, Phys.Rev.B. 49: 14251.