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Željko Šljivančanin
Srdjan Stavrić and Zoran S. Popović
University of Belgrade, Vinča Institute of Nuclear Sciences, P.O.Box 522, 11001 Belgrade, Serbia

zeljko@vinca.rs

Ab-initio modeling of metal interaction with 2D materials

Employing density functional theory we studied microscopic mechanisms governing binding of metal atoms and their nanostructures at selected 2D materials. First, we considered Li interaction with monolayers of several transition metal oxides and dichalcogenides, carbides of group XIV elements, functionalized graphene, silicene and germanene, as well as black phosphorus and Ti_2C MXene. We found that the general trend in Li binding can be estimated from positions of conduction band minima of 2D materials, since the energy of the lowest empty electronic states shows a nice correlation with the strength of Li adsorption [1]. At variance to the majority of studied surfaces where occurs a simple electron transfer from Li to the substrate, in monolayers of carbides of group XIV elements Li adsorbates profoundly modify substrates, creating well-localized mid-gap states. The second part of presented work describes growth mode of Li, Ti and Ca on graphene [2] and structural and electronic properties of graphene/MoS_2 heterostructure intercalated with Au [3]. The tendency towards the planar or three-dimensional growth of metals on graphene is rationalized based on the atomic-scale description of the interaction between metal adatoms, as well as adsorption geometries of their smallest nanostructures on graphene [2]. Finally, we show that graphene/MoS_2 represents a suitable template to produce a quasi-free-standing 2D Au monolayer with the electrons in the vicinity of Fermi level closely resembling features of 2D free electron gas [3].

References

[1] S. Stavrić, Z. S. Popović and Ž. Šljivančanin, Physical Review Materials (accepted for publication)
[2] S. Stavrić, M. Belić and Ž. Šljivančanin, *Carbon* **96** (2016), 216.
[3] Ž. Šljivančanin and M. Belić, Physical Review Materials **1** (2017), 044003.

Figures

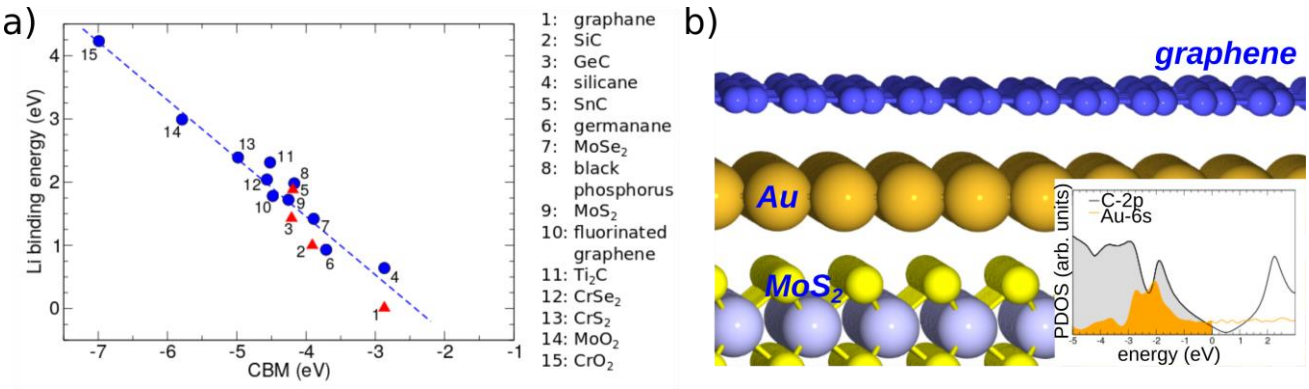

Figure 1: a) Correlation between Li binding energy and conduction band minimum (CBM) of studied 2D materials; b) atomic structure and (inset) density of electronic states of graphene/MoS_2 intercalated with Au monolayer.