Understanding trends in lithium binding at two-dimensional materials

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Layered structure and peculiar electronic properties of two-dimensional (2D) materials foster the concept of utilizing them as main components of lithium-ion batteries. Understanding basic physical mechanisms governing the interaction of Li with 2D crystals is of key importance to succeeding in a rational design of cathode and anode materials with superior functionalities. Study of Li atoms adsorbed at graphene clearly shows that Li atoms, featuring a long-ranged electrostatic repulsion, are individually dispersed across the surface [1]. This was a motivation for the further investigation of Li adsorption at a number of different 2D materials. In this study density functional theory was applied to reveal the microscopic picture of Li interaction with 15 2D crystals, including 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 [2]. 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. At variance to the majority of studied surfaces where the electron transferred from Li is spread across the substrate, in monolayers of carbides of Group XIV elements the interaction with Li and the charge transfer are well localized. This gives rise to their capability to accommodate Li structures with a nearly constant binding energy of alkaline atoms over Li coverages ranging from well-separated adatoms to a full monolayer.

References

[1] S. Stavrić, M. Belić, Ž. Šljivančanin Carbon, 96 (2016) 216
[2] S. Stavrić, Z. S. Popović, Ž. Šljivančanin Phys. Rev. Mater., 2 (2018), 11407

Figures

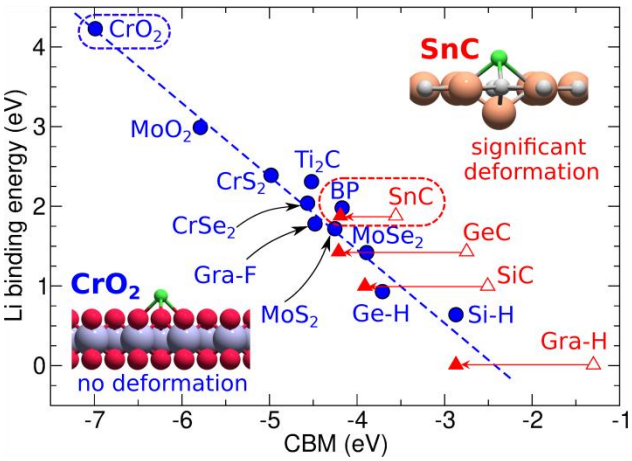

Figure 1: Correlation between Li atom binding energy (E_B) and conduction band minimum (CBM) for selected 2D crystals; 2D crystals can be divided into two groups - surfaces without (blue circles) and with the midgap state (red triangles) induced upon Li adsorption. Arrows indicate energy shifts from CBM to the energies of midgap states for the surfaces from the second group. Side view of Li atom adsorbed at the groups' representatives are also presented in the bottom left (CrO_2) and upper right corner (SnC) of the figure. The dashed line serves as a guide to eyes.