Dense storage of alkali metals between graphene and MoS2 bilayers: a computational study

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We study the intercalation of alkali metals, namely lithium and sodium, between graphene and MoS_2 sheets using density functional theory calculations with the van der Waals correction. The structures and energetics of a different number of alkali layers with closed packed structure have been investigated for various stacking sequences of bilayer graphene. The intercalation energies suggested that the AA stacking is more favorable for the single-layer intercalation but it has no considerable effect on multilayer storage. Our calculations showed that there is a clear correlation between the intercalation energy and the electron transfer between alkali atoms and layered material. While the higher values of charge transfer observed for the single layer intercalation, the charge transfer is noticeable only for the outer alkali layers in the multi-layer case. As a result, the intercalation energy reduces with increasing the number of the lithium and sodium layers but r educes f or potassium. In the case of lithium intercalation between MoS_2 bilayers, a 2H-1T phase transition was observed due to the significant charge transfer. The present study can shed light on the design of high storage alkali batteries using two-dimensional layered materials as reported recently [1].

[1] M. Kühne, F. Börrnert, S. Fecher, M. Ghorbani-Asl, J. Biskupek, D. Samuelis, A. V. Krasheninnikov, U. Kaiser, J. H. Smet, *Nature* **564**, 234-239 (2018).