Correlation of van der Waals Binding Energy of Layered Materials and Their Bulk Modulus

Mohsen Moazzami Gudarzi
National Graphene Institute, University of Manchester, Booth St. E, M13 9PL, Manchester, UK
Mohsen.moazzamigudarzi@manchester.ac.uk

Lifshitz's theory has been successfully used to compute the magnitude of vdW interactions among materials [1]. The challenge is that this theory needs the full spectrum of dielectric function of materials which is not always available [2]. When materials are optically anisotropic, the challenge is twofold, because dielectric functions along all optical axes are required [2]. I presented an argument on how to reliably derive these functions based on the limited optical properties available for layered materials. This approach allows to construct the dielectric functions of a large number of layered materials and to estimate the magnitude of their vdW binding energies. The computed binding energies for non-polar layered materials showed good agreement with rigorous *ab*-initial calculations [3,4] (Figure 1a). Also, a linear correlation between the calculated binding energies and the reported bulk modulus of layered materials is found (Figure 1b). For 'soft' layered materials such metal halides the binding energy is low. Whereas, the oddly high binding energy reported for $PdTe_2$ [3,4] manifests itself in a very large bulk modulus [5]. Based on these observations, it is proposed that the widely reported PVT equation of states of layered materials can be used to assess the binding energy. For instance, it is expected that the binding energy of graphite is lower than MoS_2 and hBN's is lower than both.

References

[1] I.E. Dzyaloshinskii , E.M. Lifshitz and L.P. Pitaevskii, Adv. Phys., 10 (1961) 165-209
[2] L. M. Woods et al., Rev. Mod. Phys., 88 (2016) 045003
[3] T. Björkman, A. Gulans, A. V. Krasheninnikov, and R. M. Nieminen, Phys. Rev. Lett., 108 (2012) 235502
[4] N. Mounet et al., Nature Nanotech., 13 (2018) 246-252
[5] C. Soulard et al., J. Solid State Chem., 178 (2005) 2008-2014

Figures

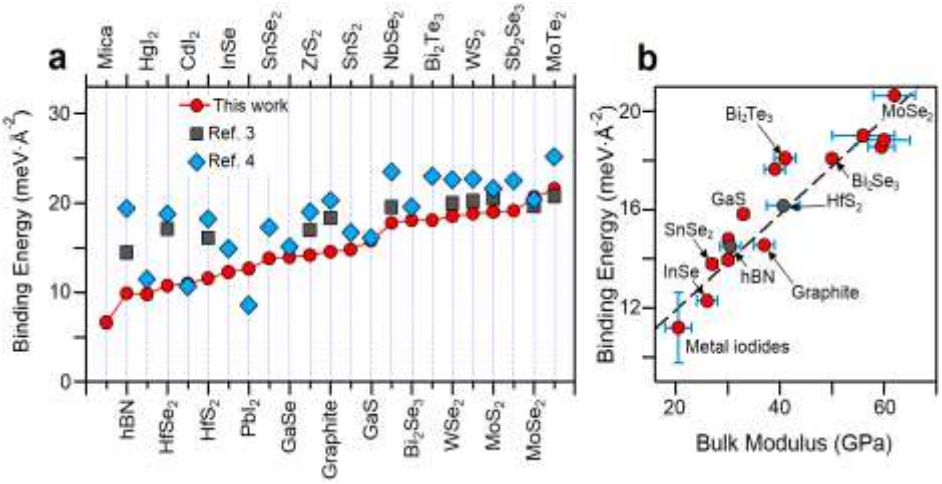

Figure 1: (a) Computed binding energies of different layered materials. For non-polar materials where layers are held together by mostly vdW interactions, there is good agreement between this study and Ref. [3]. For polar materials such as hBN, additional non-vdW interactions exists. (b) Binding energy versus bulk modulus of 16 different layered materials. For polar layered materials (hBN and HfS_2) contribution of non-vdW interactions should be taken into account for them to follow other layered materials. Therefore, data of Ref. [3] are used for these two materials.