London Dispersion Corrected DFT and its Impacts on Electronic Band Structure Calculations

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It must be a twist of fate that Sir Isaac Newton developed the foundations of classical mechanics by unwittingly using the quantum mechanical London dispersion interactions thanks to his pencil. However, graphene layers of the pencil are not the only layers that hold together by London dispersion interactions. A wide spectrum of layered materials exist, and novel properties of their single or few layers got the attention of scientists due to their novel properties. To reveal these novel properties, London dispersion interactions also needed to be taken into account properly in addition to the other electromagnetic interactions. In the Density Functional Theory (DFT) formalism, these interactions are not included in the standard DFT functionals due to their local and semi-local natures [1,2]. In this study, we showed the computationally affordable PBE-rVV10L non-local DFT functional is predicting London dispersion interaction governed interlayer distances and interlayer interaction energies of eighteen bulk layered systems with mean absolute errors (MAE) of 0.092 Å and 3.25 meV/atom, respectively. In addition to this, we revealed the importance of the interlayer distances on electronic band structure calculations.

References

[1] S. Grimme, Wiley Interdiscip. Rev. Mol. Sci., 1 (2011) 211-228
[2] G.R. Bhimanapati, Z. Lin, V. Meunier, Y. Jung, J. Cha, S. Das, Di Xiao et al., ACS Nano, 9 (2015) 11509-11539

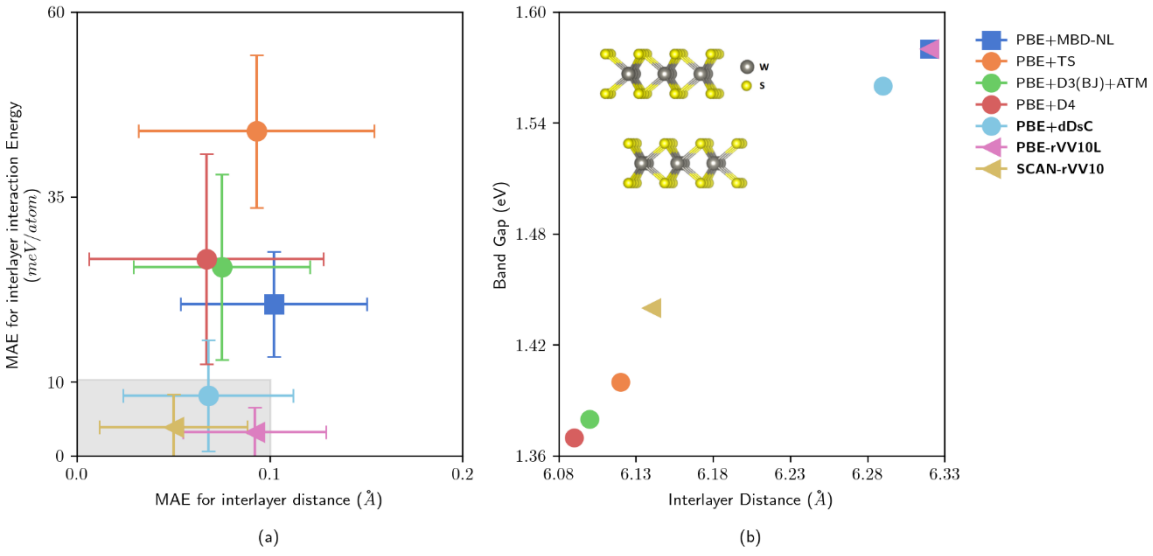

Figure 1: (a) Interlayer distance and interlayer interaction energy mean absolute errors (MAE) of 18 layered bulk systems with their standard deviations for the tested methods. We took experimental interlayer distances and our Random Phase Approximation (RPA) interlayer interaction energy calculations as reference data. (b) The impact of the initial interlayer distance on the HSE06+SOC band gaps for the WS_2 bulk system. The same pattern also exists for other systems. While the x-axis shows the interlayer distances of the WS_2 bulk system determined with corresponding methods, the y-axis shows HSE06+SOC band gaps determined on top of those geometries.