Layer Response theory for semi-analytic energetics of vdW bound layered materials

John Dobson¹

1) Griffith University

Corresponding author: John Dobson (j.dobson@griffith.edu.au)

This work aims for efficient modelling of cohesive properties in soft layered materials involving graphenes, MoS2 etc. and their adsorbates. The costly Random Phase Approximation (RPA) and extensions, with the Adiabatic Connection Fluctuation Dissipation (ACFD) theorem plus groundstate exchange (EXX) seems to be the only approach that reliably gives these energies in such difficult cases as mixed graphenic and metallic layers. This difficulty is partly due to non-additive van der Waals forces that are not well modelled in less numerically demanding DFT+vdW theories. We first show how to use 3D plane-wave codes for efficient prediction of the long-wavelength dielectric response of an isolated layer, while avoiding unit cells with large vacuum gaps and the corresponding large calculations. This data is then used with the RPA/ACFD to obtain semi-analytically the cohesive energetics involving such layers with other layers and molecular entities. Insulating, metallic and graphenic layers are all treated with correct asymptotic and sub-asymptotic van der Waals behavior. The inner parts of the interaction energy curve can be matched to efficient calculations using semi-local density functionals. We recently applied this approach to a water molecule on graphene, economically recovering results previously obtained from extremely large full RPA correlation calculations.