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TÉMA

An accurate DFT-based method for the treatment of weak and van der Waals interactions : the LCAO-S2+vdW formalism

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Strong developments in nanomolecular systems have reinforced the importance of weak and van der Waals interactions. Standard Density Functional Theory (DFT) is unable to describe correctly these kind of interactions. This is mainly due to the local character of the standard functional approximations (LDA,GGA, ...), in opposition with the long range behaviour of the van der Waals interaction.
In this presentation, I will mainly focus on the important role played by weak interactions-among them the so called van der Waals interaction-in Carbon based Nanostructures, like the interaction between two graphene sheets for example. These interactions are fundamental to the stability of such structures. Here we present a DFT based formalism, the LCAO-S2+vdW method, which is an intermolecular perturbation theory coupled with the use of the dipolar approximation, in order to treat weak and van der Waals interactions. This method has already been applied giving good results to the study of graphene-graphene interaction [1], and to more graphitic materials like Carbon Nanotubes or fullerenes [2]. I will detail these results and present some new perspectives for molecular Hydrogene dimer and adsorption on Carbon Nanotubes.

[1] Y. J. Dappe, M. A. Basanta, F. Flores, and J. Ortega, Phys. Rev. B 74,205434 (2006).
[2] Y. J. Dappe, J. Ortega, and F. Flores, Phys. Rev. B 79, 165409 (2009).

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