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Self-consistent van der Waals density functional: Development and Applications

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The inability of density functional theory (DFT), with standard exchange-correlation functionals, to correctly describe van der Waals/dispersion (vdW) interactions has severely limited its applicability to sparsely packed systems, such as organic and biological molecules. Numerous attempts have been made to correct these deficiencies; however, many of them either require extensive reparameterization for each new situation or scale poorly with system size. In this paper, I will discuss the development and implementation of an exchange-correlation functional which correctly incorporates non-local vdW interactions within DFT (vdW-DF)[1]. In addition, I will present our recent development of the corresponding exchange-correlation potential ($V_{\rm xc}$)[2]. The $V_{\rm xc}$ gives us the ability to compute Hellmann-Feynman forces, allowing for structural relaxations and molecular dynamics simulation. Using the $V_{\rm xc}$ I will examine the nature of the van der Waals bond between molecules. Finally, to demonstrate the power of the vdW-DF, I will discuss our relatively large scale application of the functional to study the influence of stacking interactions on the structure and stability of DNA. Here, I will show how these interactions are crucial for defining the twist and base pair separation in DNA and how methyl-nucleobase and methyl-methyl interactions give additional stability to DNA.

[1]M. Dion, H. Rydberg, E. Schröder, B. I. Lundqvist and D. C. Langreth, Phys. Rev. Lett., **92**, 246401 (2004)
[2]T. Thonhauser, V. R. Cooper, S. Li, A. Puzder, P. Hyldgaard, and David C. Langreth, Phys. Rev. B, **76**, 125112 (2007)