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 (\(V_{xc}\))\(^2\). The \(V_{xc}\) gives us the ability to compute Hellmann-Feynman forces, allowing for structural relaxations and molecular dynamics simulation. Using the \(V_{xc}\) 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.
