Applications of the van der Waals density functional to DNA and metal organic framework materials

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The inability of density functional theory, with standard exchange correlation functionals, to correctly describe van der Waals/dispersion interactions has severely limited its applicability to sparsely packed systems, such as organic and biological molecules. Here, I will discuss our application of the recently developed van der Waals density functional[1,2] to study the influence of stacking interactions on the structure and stability of DNA[3,4] and to simulate the interactions of H_2 within metal-organic framework (MOF) materials. Our results for base pair stacking interactions demonstrate that 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. In regards to the MOF we show that modeling the entire MOF structure can result in different H_2 adsorption geometries, binding energies and vibrational frequencies than observed in previous calculations on fragments of the MOF. Combining these results with experimental IR vibrational frequency studies should provide insights into modifying MOF structure and composition for enhanced H_2 uptake.

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