Capturing van der Waals Interactions in DFT Through Non-Local Exchange and Correlation

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We discuss the development of the truly non-local exchange-correlation van der Waals density functional (vdW-DF) [1], which can reliably capture van der Waals interactions in density functional theory. We start by giving a historical overview, including earlier attempts to capture van der Waals interactions through non-locality. Thereafter, we give a formal derivation of the vdW-DF functional, highlighting its firm foundation in many-body perturbation theory through the adiabatic coupling fluctuation dissipation theorem [2, 3]. In this context, we also discuss recent developments such as the inclusion of spin [4] and the development of more accurate and promising variants. Finally, we show a selected subset of applications where vdW-DF has been crucial to uncover important mechanisms and processes in physics and chemistry, focusing on hydrogen storage and small molecule adsorption in metal organic framework materials.

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