Accurate van-der-Waals interactions from (semi)-local density functional theory ALEXANDRE TKATCHENKO, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG, Berlin, Germany — Non-covalent forces, such as hydrogen bonding and van der Waals (vdW) interactions, are crucial for the formation, stability and function of molecules and materials. At present, vdW interactions can only be satisfactorily accounted for by high-level quantum-chemical wave function or by the Quantum Monte Carlo (QMC) method. In contrast, (semi)-local DFT and Hartree-Fock approximation fail for the description of vdW forces. We present a parameter-free method for describing the long-range vdW interaction in (semi)-local DFT. The leading C_6 coefficients are derived from the electron density of a molecule/solid and accurate reference values for the free atoms. The mean absolute error in the C_6 coefficients is 5.5% when compared to accurate experimental values for 1225 intermolecular pairs. We show that the C_6 coefficients depend strongly on the bonding type and geometry of molecules/solids. Finally, we analyze the vdW radii and the damping function in the $C_6 R^{-6}$ correction method for DFT calculations.

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