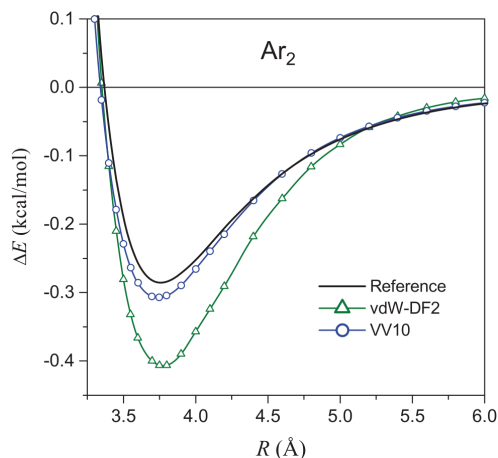
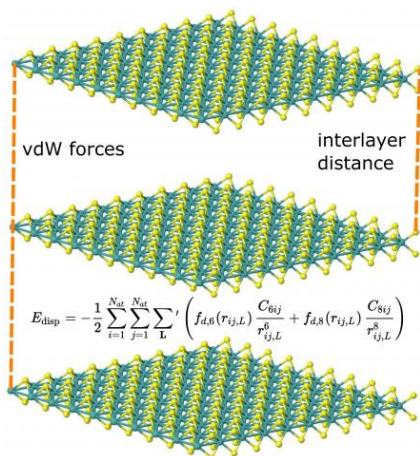


Dispersion Correction in Density Functional Theory

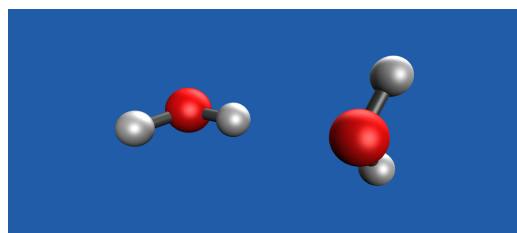


Dispersion (van der Waals) interaction plays a crucial role in the formation, stability, and function of molecules and materials. However, long-range correlation, which is the physical root of dispersion interaction, is absent in popular local or semi-local exchange-correlation functionals. Thus, proper dispersion corrections are necessary for DFT calculations on realistic systems. Q-Chem offers several theoretical models for dispersion correction, at a negligible computational overhead compared to standard DFT:

- Non-local correlation functional: e.g., the VV10 functional;
- Empirical dispersion correction of Grimme (the DFT-Dx series): DFT-D2, DFT-D3, DFT-D4, etc;
- Exchange-dipole model of Johnson and Becke (XDM);
- Tkatchenko-Scheffler van der Waals model (TS-vdW);
- Many-body dispersion (MBD) method.

H-bond Energy (kJ/mol)

CCSD(T)	21.5
wB97x-D4	24.5
wB97x-D3	28.0



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