Q-CHEM

A Quantum Leap Into the Future of Chemistry

What's New in Q-Chem

The Dispersion Correction of DFT with XDM Model

Developers: Zhengting Gan and Emil Proynov

The dispersion is an important interaction that has been missing in current DFT functional. Q-Chem developers have implemented a correction based on Becke and Johnson's exchange dipole moment (XDM) model. Unlike empirical classic correction that is MM-like, XDM is a density-functional model with few empirical parameters. Including XDM in the DFT calculation adds little to the computational cost. This feature should be included in all calculations of molecular structures, large or small.

For more information on how to use this feature, refer to the Q-Chem Manual, Section 4.3.5.

Publication: J. Kong, Z. Gan, E. Proynov, M. Freindorf, T.R. Fulani, "Efficient computation of the dispersion interaction with density-functional theory", Phys. Rev. A **79** 042510 (2009).

Emil Proynov

Zhengting Gan

MP2 **B3LYP** **B3LYP-XDM**

Geometries of tyrosine-glycine dipeptide obtained using 6-31+G* basis set

The illustration shows that XDM makes a qualitative improvement in the prediction of the molecular structure. The first dipeptide, which has a closed-book conformation, is calculated with the MP2 method, a wave-function-based method that includes dispersion. The second structure is calculated with B3LYP, a popular DFT method, which has an incorrect open-book structure. The third structure is calculated with B3LYP with XDM correction, which qualitatively agrees with MP2. Note that the energy correction is 8 kcal/mol, a very significant amount.

For see more new features, visit:
www.q-chem.com/whatsNew4.html

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