

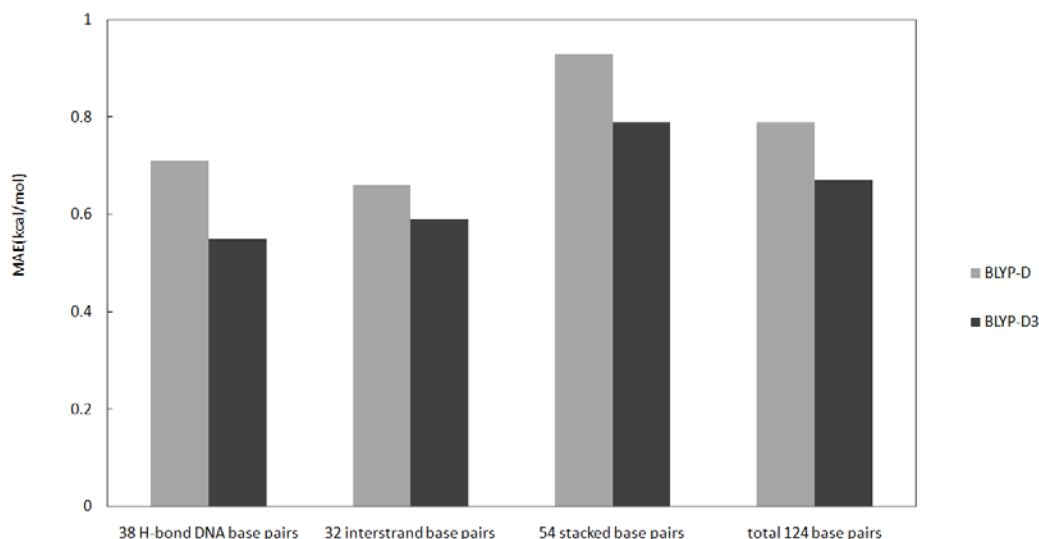
## What's New in Q-Chem

Feature 15

### DFT-D3 Methods

**Developers:** Shan-Ping Mao and Jeng-Da Chai

The conventional DFT functionals usually lack for the dispersion interactions. We have implemented a new method of dispersion correction (DFT-D3) that was developed by Grimme and co-workers. The important improvements of the new method are the dispersion coefficients and cut of radii which are less empirical and both computed from first principle. 3 body terms in dispersions can be included. It should be included in the calculations of noncovalent systems.



This graph shows that the binding energies of 124 nucleic acid pairs in JSCH-2005 set are calculated by BLYP-D and BLYP-D3 with 6-311++G(3df,3pd) basis set. For all the subsets (H-bond DNA, interstrand and stacked base pairs), BLYP-D3 has the more accurate mean absolute errors (MSEs) than BLYP-D. We significantly notice the MAE reduction of H-bond DNA base pairs about 35%, and the MAE of the total 124 base pairs is reduced from 0.79 to 0.67(kcal/mol).

For more new features, visit:

[www.q-chem.com/whatsNew4.html](http://www.q-chem.com/whatsNew4.html)

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The Design Center, Suite 690 • 5001 Baum Boulevard • Pittsburgh, Pennsylvania 15213 • United States of America

Telephone: (412) 687-0695 • Facsimile: (412) 687-0698 • E-Mail: [info@q-chem.com](mailto:info@q-chem.com)

Website: <http://www.q-chem.com>

## What's New in Q-Chem

### DFT-D3 Methods (continued)



#### *Publications:*

[S. Grimme, J. Antony, S. Ehrlich, and H. Krieg, "A consistent and accurate ab initio parametrization of density functional dispersion correction \(DFT-D\) for the 94 elements H-Pu," J. Chem. Phys. \*\*132\*\*, 154104, \(2010\)](#)

For more information on how to use this feature, refer to the [Q-Chem Manual, Section 4.3.7](#).

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