What's New in Q-Chem

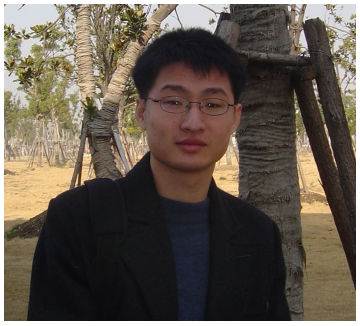
Fast OS Doubly Hybrid Density Functional Close to Chemical Accuracy

Developers: Igor Ying Zhang, Xin Xu, Yousung Jung and Bill Goddard

This feature, XYGJ-OS, is a doubly hybrid density functional whose accuracy is close to doing chemistry (MAD: 1.5 kcal/mol) with the fast algorithm that scales cubically with system size due to opposite-spin ansatz. It has both the accuracy comparable to the G3 theory and the speed that can be applicable to large systems due to a cubic scaling algorithm instead of fifth order in other doubly hybrid functionals. XYGJ-OS is very effective for calculating energies.

Publication: Igor Ying Zhang, Xin Xu, Yousung Jung, Bill Goddard, *"[actual title of article here]"*

[submitted-insert reference w/link here]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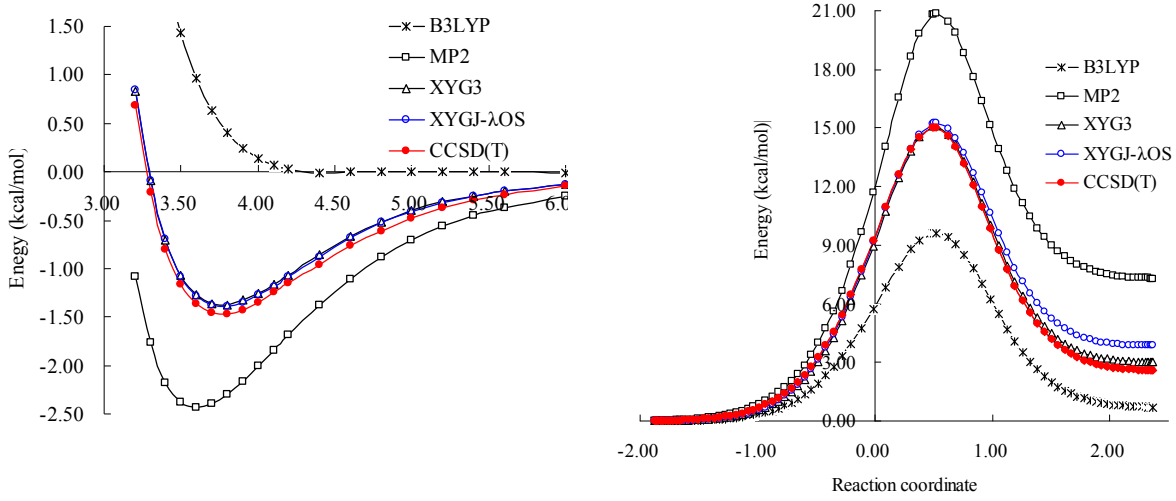
What's New in Q-Chem

Fast OS Doubly Hybrid Density Functional Close to Chemical Accuracy) (continued)

The figures show the potential energy curve of the H + CH_4 → H_2 + CH_3 reaction (left), and the intermolecular potentials for the CH_4-C_6H_6 complexes (right) from various methods where R is defined as carbon of CH_4 to the ring center of C_6H_6 (in Å). It is remarkable that XYGJ-OS yields the correct shapes of the potential energy surfaces close to CCSD(T), and not just accurate thermochemical single point energies.



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

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

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