

Development of the XYG3-type doubly-hybrid functionals

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The so-called doubly-hybrid density functionals (DHDFs) incorporate the information of unoccupied orbitals in the form of second order perturbation, and stay on the fifth rung of the Jacob's ladder, according to Perdew's classification [1], close to the heaven of "chemical accuracy". Being a representative of one type of DHDFs, XYG3 shows a promising performance in predicting heats of formation, bond dissociation enthalpies, reaction barrier heights, and non-bonded interactions for chemistry of the main group elements [2,3].

However, there are several issues which call for further improvements. For example, as compared to the lower rung functionals, DHDFs are computationally more demanding, being one to two orders of magnitude higher, which prohibits their application to larger systems. Meanwhile, several recent studies revealed that XYG3 still has a tendency to underestimate the van der Waals interactions.

In this presentation, some new developments for the speedup of the DHDF calculations [4] and an improved description of van der Waals interactions will be addressed [5]. As XYG3 has now been implemented in FHI-aims, a brief introduction on this new feature will also be given in the presentation.

[1] J. P. Perdew, K. Schmidt, Density functional theory and its application to materials, edited by V. V Doren, 2000

[2] Y. Zhang, X. Xu and W. A. Goddard III, Proc. Nat. Acad. Sci. USA, 106(2009) 4963

[3] I. Y. Zhang, and X. Xu Int. Rev. Phys. Chem. 30(2011) 115

[4] I. Y. Zhang, X. Xu, Y. Jung, and W. A. Goddard III, Proc. Nat. Acad. Sci USA, 108(50)(2011)19896.

[5] I. Y. Zhang, X. Xu, to be published.