Università degli Studi di Torino
Dipartimento di Chimica
Via P. Giuria, 7 10125 Torino Italy

Avviso di Seminario

Mercoledì 22 Febbraio alle ore 14:30 presso la Sala di Rappresentanza del Dipartimento di Chimica (via P. Giuria 9) il

Prof. Xin Xu

della Fudan University di Shanghai (China)

terrà un seminario dal titolo:

"The XYG3-type of doubly hybrid density functionals"

Il responsabile scientifico

Prof. Bartolomeo Civalleri

Il Direttore del Dipartimento

Prof. Marco Vincenti

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Abstract

The XYG3-type of doubly hybrid density functionals

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Doubly hybrid (DH) functionals present a new class of density functionals, which enfold the non-local orbital-dependent components not only in the exchange part, but also in the correlation part. Different types of DH functionals have been proposed according to different philosophies [1-3], where the XYG3-type of functionals (xDH) [5-9] is unique in its framework that a conventional (general) Kohn-Sham (KS) functional, such as B3LYP or PBE0 or PBE, is utilized for the self-consistent-field (SCF) calculations to generate orbitals and density, with which a DH functional is used for the final energy evaluations.

This talk will focus on the development of the xDH functionals. (1) We will discuss the theoretical background of the xDH functionals, briefly reviewing the adiabatic connection formalism, coordinate scaling relations, and Görling–Levy perturbation theory. [1-3]. (2) A long-range-corrected XYG3 (i.e., lrc-XYG3) is presented, which includes a range-dependent term from the second order perturbation theory for better description of dispersive interaction [7]. (3) Analytic gradients are discussed, where the non-variational contributions from the SCF functional to the final energy functional are solved through a coupled-perturbed KS equation [10, 11]. (4) Fractional charge behaviours of DH functionals are explored [12], which lead to good predictions of ionization potentials, electron affinities and fundamental gaps from the perspective of fractional charges. (5) A non-fitted DH functional, namely PBE-ACDH, is constructed based on the adiabatic connection (AC) formalism, coordinate scaling relations, and the second order Görling-Levy perturbation theory [9], where contributions from density scaling and singles are explicitly considered.

Limitations of the present approaches and the direction for future improvements will be discussed.

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Curriculum Vitae

Prof. Xin Xu received his doctoral degree in theoretical chemistry from Xiamen University, China, in 1991. After a postdoctoral stay at Fujian Institute of Research on the Structure of Matter, Academia Sinica, he was appointed as an associated professor in 1993 and was promoted to a full professor in 1995 in the department of chemistry, Xiamen University, where he became the Lu-Jia-Xi Chair professor in 2006. He moved to Fudan University Shanghai as a distinguished chair professor in 2010.

Prof. Xin Xu was awarded the 10-Outstanding Young Chemists of 1995, issued by Chemical Society of China. He received reward fundings from Fok Ying Tung Foundation (Hong Kong) in 1998, from State Education Commission for Outstanding Young Professors in Chinese University in 2000, and from National Natural Science Foundation for Outstanding Young Scientists in 2006. He was appointed as a Ming-Jiang Scholar of Fujian province in 2006, and a Cheung-Kong scholar in 2012. He was a visiting professor at Kyoto University, Japan; California Institute of Technology, USA; University of Science and Technology, Hong Kong and Ecole Normale Supérieure de Lyon, France, etc. He has authored and co-authored 200 peer-reviewed papers with more than 7000 citations. He has been invited to give over 200 lectures, including “The 12th and 15th International Congress of Quantum Chemistry (2006, 2015)”. His main research area is **Density Functional Theory (DFT) and its applications**.