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NOMAD CoE Colloquium

Moderator:
Matthias Scheffler

Speaker: **Professor Weitao Yang**
Department of Chemistry and Department of Physics
Duke University, USA

Topic: **Density Functional Theory: Correcting Systematic Errors and Predicting Photoemission and Photoexcitation Spectroscopy from Ground State Calculations**

Date, time: Thursday, November 10, 2022 at 16:15 CET
We meet at 15:45 CET in front of the lecture hall for coffee, tea, and cakes.

Location: Lecture hall 0'119 at Erwin Schrödinger Zentrum (ESZ), Rudower Chaussee 26, 12489 Berlin – Adlershof (in-person participation is preferred!)

For participation via zoom, please register via the following registration webpage:
https://gmogni.aidaform.com/NOMAD-CoE-Colloquium

Abstract:

The systematic delocalization and static correlation errors in DFT, based on the fractional analysis, underlie many challenges in density functional theory calculations. To eliminate these two errors, we developed a localized orbital scaling correction (LOSC): it accurately characterizes the distributions of global and local fractional electrons and spins, and is thus capable of correcting system energy, energy derivative and electron density in a size-consistent manner. Our approach introduces the explicit derivative discontinuity and largely restores the flat-plane behavior of electronic energy at fractional charges and fractional spins. The LOSC–DFAs lead to systematically improved results, including the dissociation of ionic species, single bonds, multiple bonds without breaking the space or spin symmetry, the band gaps of molecules and polymer chains, the energy and density changes upon electron addition and removal, and photoemission spectra, and energy-level alignments for interfaces. The LOSC DFA

orbital energies are excellent approximations to quasiparticle energies, comparable to or better than GW. This also leads to the QE-DFT (quasiparticle energies from DFT) approach: the calculations of excitation energies of the N-electron systems from the ground state DFA calculations of the (N - 1)-electron systems. Results show good performance with accuracy similar to TDDFT for valence excitations with commonly used DFAs with or without LOSC. For charge transfer and Rydberg states, good accuracy was obtained only with the use of LOSC DFA. The QE-DFT method has been further developed to describe excited-state potential energy surfaces (PESs), conical intersections, and the analytical gradients of excited-state PESs. We have also made the LOSC software available for the community.

References

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