Special Seminar

Presented by

Dr. Yang Yang

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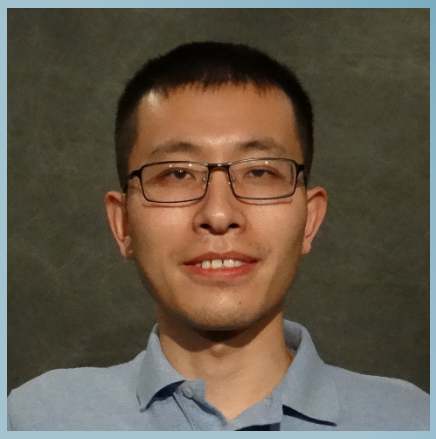

"Multicomponent Density Functional Theory and Time-Dependent Density Functional Theory Based on Nuclear-Electronic Orbital Approach"

The quantum mechanical treatment of both electrons and protons in the calculation of ground and excited state properties is critical for describing nonadiabatic processes such as proton-coupled electron transfer. Multicomponent density functional theory (DFT) enables the consistent quantum mechanical treatment of more than one type of particle. An electron-proton correlation functional, epc17, was derived analogously to the Colle-Salvetti formalism for electron correlation and implemented within the nuclear-electronic orbital (NEO) framework. The NEO-DFT/epc17 method produces accurate proton densities and proton affinities. The linear response multicomponent time-dependent density functional theory (TDDFT) was also derived and implemented. Initial applications illustrate that NEO-TDDFT provides accurate proton and electron excitation energies within a single calculation. The NEO-DFT and NEO-TDDFT methods are promising for diverse applications, particularly nonadiabatic proton transfer reactions.

Monday, January 14 at 3:30 p.m. in 1315 Chemistry