The Density-Based Reactivity Theory

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Abstract

Density functional theory well-recognized by its accuracy and efficiency has become the workhorse for modeling the electronic structure of molecules and extended materials in the past decades. Nevertheless, how to establish a density-based conceptual framework to appreciate bonding, stability, function, reactivity, and other physicochemical properties is still an unaccomplished task. In this talk, we at first overview the four pathways currently available in the literature to tackle the matter, including orbital-free density functional theory, conceptual density functional theory, direct use of density associated quantities, and information-theoretic approach. Then, we highlight several recent advances of employing these approaches to harvest new understandings for chemical concepts such as covalent bonding, noncovalent interactions, cooperation, frustration, homochirality, chirality hierarchy, electrophilicity, nucleophilicity, regioselectivity, and stereoselectivity. Finally, we provide a few outlooks for the future development of this relatively uncharted territory.

Biography

Dr Shubin Liu is a Senior Computational Scientist at the Research Computing Center and an Adjunct Professor at the Department of Chemistry, University of North Carolina at Chapel Hill. He obtained his Ph.D. degree with Robert G. Parr in 1996 and finished postdoctoral training with Weitao Yang of Duke University. He has been an independent researcher at the University of North Carolina since 2000, focusing on developing a chemical reactivity theory using density functional theory language. Dr. Shubin Liu has co/authored over 270 peer-reviewed publications with h-index of 60 and is recognized in the field by various scientific awards including the Wiley-IJQC Young Investigator Award.