Development and Applications of Density-Based Theory of Chemical Reactivity

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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. Opportunities are abundant, and they are all ours for the taking.