Information-Theoretic Approach in Density Functional Reactivity Theory

Shubin Liu

Research Computing Center, University of North Carolina,
Chapel Hill, North Carolina 27599-3420

Density functional reactivity theory (DFRT) is a recent endeavor to appreciate and quantify molecular reactivity with simple density functionals. Examples of such density functionals recently investigated in the literature included Shannon entropy, Fisher information, and other quantities from information theory. This work presents an overview on the principles of the information-theoretic approach in DFRT, including the extreme physical information principle, minimum information gain principle, and information conservation principle. Three representations of this approach with electron density, shape function, and atoms-in-molecules partition are also summarized. Moreover, their applications in quantifying steric effect, electrophilicity, nucleophilicity, and regioselectivity are highlighted, so are the recent results in a completely new understanding about the nature and origin of *ortho/para* and *meta* group directing phenomena in electrophilic aromatic substitution reactions. A brief outlook of a few possible future developments is discussed at the end.