Exploring Chemical Reactivity based on Conceptual DFT and Quantum Chemical Topology coupling

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This contribution presents a mechanistic methodology designed to identify the favourable reaction pathway between reactants at low computational cost. The methodology draws on the conceptual Density Functional Theory [1] and the quantum chemical topology approach. [2] Two different descriptors will be presented. The first relies on the difference between the local interacting chemical potentials [3] of the reactants in agreement with the Sanderson's equalization principle. [4] The second approach uses the so-called dual descriptor condensed over the ELF topological domains. [5] Illustrative examples will be provided for non-covalent donor-acceptor systems as well as for some reactive systems. Finally, the strengths and limitations of the presented approaches in predicting chemical reactivity will be outlined.

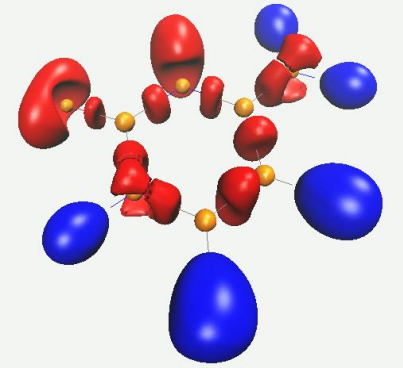

Figure 1. Condensed dual descriptor in ELF domains for the guanine. Color code: blue: electrophilic, red nucleophilic, orange : aphilic.

References.

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[4] Sanderson, R. T., *Science* **1955,** *121* (3137), 207-208.
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