Chemical Reactivity Indicators When There Is Strong Electron Correlation

Paul W. Ayers, Michelle Richer, Gabriela Sanchez-Diaz

*Department of Chemistry & Chemical Biology; McMaster University*

*ayers@mcmaster.ca*

Many conceptual tools for interpreting molecular structure and reactivity are tethered to the orbital picture; even those which are not are typically evaluated using uncorrelated wavefunction methods. The former issue is resolved by developing conceptual tools that are based on physical observables [1]. We show how (di)radical-based and spin-based reactivity can be robustly treated in the framework of conceptual density functional theory, and evaluate the resulting indicators using both traditional Kohn-Sham density-functional theory methods and near-exact *ab initio* approaches. The equation-of-motion strategy can be used to compute conceptual density functional theory reactivity indicators in the framework of *ab initio* approaches.

[1] P. W. Ayers, S. Fias, and F. Heidar-Zadeh. “The axiomatic approach to chemical concepts”. *Computational and Theoretical Chemistry* 1142 (2019), pp. 83–87. DOI: 10.1016/j.comptc.2018.09.006.