

Conceptual DFT and Higher-Order Quantum Reactivity Descriptors

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Conceptual Density Functional Theory (Conceptual DFT) provides a powerful framework for understanding and predicting chemical reactivity through quantum reactivity descriptors. In this presentation, I will discuss the importance of these descriptors and their role in rationalizing chemical behavior. Particular attention will be given to our recent work, where we extended reactivity descriptors up to the fourth order. These developments offer new insights into electronic structure, response properties, and chemical reactivity, opening promising perspectives for theoretical and computational studies.