Exploring The Reactivity of Donor-Acceptor Systems Through a Combined Conceptual and Constrained DFT Approach

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ABSTRACT

In this contribution we show, in the context of the conceptual Density Functional Theory [1] and based on the computational efficiency of the constrained DFT [2], that chemical reactivity can be governed by the difference between the local interacting chemical potentials [3, 4] of the reactants in agreement with the Sanderson's equalization principle. Illustrative examples will be given involving non-covalent donor-acceptor systems as well as for reactive systems. For the selected systems, the approach reveals a significant mimicking between the proposed descriptor and the DFT-calculated intermolecular interaction energy profiles. [5,6] Finally, the strengths and limitations of the presented Sanderson-like model in predicting chemical reactivity will be outlined.

References

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