Reactivity Indices in Density Functional Softness Theory

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The chemical space of the reactivity by means of the density functional theory definitions of electronegativity (χ) and of chemical hardness (η) is introduced through the orthogonality realization of "level $\perp$ interval" (for the semi-sum and the semi-difference of the highest occupied HOMO and the lowest unoccupied LUMO molecular orbitals) around the (global) equilibrium of the total energy (E_N) parabolically depending on the system's electrons (or the valence electrons). Such "orthogonal" interpretation ($\chi \perp \eta$) is confirmed by the *cutting observable* (χ) *vs. indeterminate observable* (η) characters as proved by the second quantification approach. This dichotomy justifies the development of the atomic radii scales (without observable operator in quantum physics) through employing electronegativity as observable chemical quantity, and later implemented for chemical hardness and adjacent quantities (as diamagnetic susceptibility, polarizability) as indirect-observable structural properties. Finally, a new formulation and classification of the hard-hard, soft-soft and hard-soft reactivity behavior was realized through introducing the maximum chemical hardness index (Y) by the orthogonal completing relationship

$$1 = \frac{S}{\eta} + \mathrm{Y}$$

Selected References

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