



Chemical Reactivity Theory: A Density Functional View

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In the 1970s, Density Functional Theory (DFT) was borrowed from physics and adapted to chemistry by a handful of visionaries. Now chemical DFT is a diverse and rapidly growing field, its progress fueled by numerous developing practical descriptors that make DFT as useful as it is vast. With 34 chapters written by 65 eminent scientists from 13 different countries, **Chemical Reactivity Theory: A Density Functional View** represents the true collaborative spirit and excitement of purpose engendered by the study and use of DFT.

This work instructs readers on how concepts from DFT can be used to describe, understand, and predict chemical reactivity. Prior knowledge is not required as early chapters, written by the field's original pioneers, cover basic ground-state DFT and its extensions to time-dependent systems, excited states, and spin-polarized molecules. While the text is accessible to senior undergraduate or beginning graduate students, experienced researchers are certain to find interesting new insights in the perspectives presented by these seasoned experts. This remarkable one-of-a-kind resource—

- Provides authoritative accounts on aspects of the theory of chemical reactivity
- Describes various global reactivity descriptors, such as electronegativity, hardness, and electrophilicity
- Introduces and analyzes the usefulness of local reactivity descriptors such as Fukui, shape, and electron localization functions
- Offers an in-depth analysis of how chemical reactivity changes during different physicochemical processes or in the presence of external perturbations

The book covers a gamut of related topics such as methods for determining atoms-in-molecules, population analysis, electrostatic potential, molecular quantum similarity, aromaticity, and biological activity. It also discusses the role of reactivity concepts in industrial and other practical applications. Whether you are searching for new products or new research projects, this is the ultimate guide for understanding chemical reactivity.

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