






Chapter 14 - On the analysis of the Fukui function

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<https://doi.org/10.1016/B978-0-32-390257-1.00021-8> 

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Abstract

In this chapter we review the fundamentals and some applications of the Fukui Function. This was defined almost 40 years ago by Robert Parr in a fantastic example of how density-functional-theory provides a formal framework for chemical reactivity concepts. The Fukui function is a generalization of Fukui's work on the regions of a molecule that are most likely to transfer electrons, and therefore most reactive.

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