

# Why is the dual descriptor a more accurate local reactivity descriptor than Fukui functions?

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A mathematical analysis reveals that dual descriptor is a more accurate tool than nucleophilic and electrophilic Fukui functions. Although Fukui function has the capability of revealing nucleophilic and electrophilic regions on a molecule, the dual descriptor is able to unambiguously expose truly nucleophilic and electrophilic regions, but along with the latter, dual descriptor is less affected by the lack of relaxation terms than the Fukui function when the frontier molecular orbital approximation is applied. This implies that the dual descriptor can be considered a more reliable descriptor to measure local reactivity than Fukui function. This statement is demonstrated in the present work. © 2014, Springer International Publishing Switzerland.

Dual descriptor

Electrophilic Fukui function

Local reactivity descriptor

Nucleophilic Fukui function