

In pursuit of negative Fukui functions: Molecules with very small band gaps

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A justification for the likely presence of negative Fukui functions in molecules with small band gaps is given, and a computational study performed to check whether molecules with small band gaps have negative Fukui functions to a chemically significant extent is reported. While regions with negative Fukui functions were observed, significantly negative values for the atom-condensed Fukui functions were not observed. © 2014 Springer-Verlag.