



Theoretical and Computational Research in the 21st Century

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The book discusses the fact that the largest and smallest values of the fukui function and local softness do not necessarily correspond to the softness and hardness regions of the molecules such as porphyrins. The authors have adopted two popular calculation procedures for this venture. One is the very old Hückel molecular orbital calculation, and the other is one of best semi-empirical AM-1 procedures for such systems. Our finding is that neither the fukui functions nor the local softnesses can predict the preferred donor sites of porphyrins toward metal ions.

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