
Chemical Reactivity Theory A Density Functional View

English Edition By Pratim Kumar Chattaraj

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May 27th, 2020 - as a continuation of our recent efforts to quantify chemical reactivity with quantities from the information theoretic approach within the framework of density functional reactivity theory the effectiveness of applying these quantities to quantify electrophilicity for the bimolecular nucleophilic substitution s n 2 reactions in both gas phase and aqueous solvent is presented in this work"fukui function

May 29th, 2020 - the condensed fukui function or condensed reactivity indicator is the same idea but applied to an atom within a molecule rather than a point in three dimensional space the fukui function allows one to predict using density functional theory where the most electrophilic and nucleophilic sites of a molecule are"**chemical reactivity theory a density functional view**

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