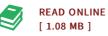# Contributions Within Density Functional Theory with Applications in Chemical Reactivity Theory and Electronegativity

By Mihai V Putz

DISSERTATION.COM, United States, 2003. Paperback. Book Condition: New. 246 x 189 mm. Language: English Brand New Book ***** Print on Demand *****.In the limits of the density functional theory there are introduced and deduced fundamental chemical descriptors as the chemical action concept, the chemical field, new electronegativity, rate reaction and chemical hardness formulations, the reduced total energy and the partial Hohenberg-Kohn functionals. For electronic density computations the quantum statistic picture of the path integral Feynman-Kleinert formalism is employed to its markovian approximation, providing the framework in which the majority of the chemical reactions and the reactivity of the electronic systems can be treated together with the internal and environmental couplings. Evaluation, representation and interpretation of the present analyzed chemical indices are performed for a prototype many-electronic system such that its electronic structure to display fundamental and excited anharmonic vibrations being in the thermal coupling with the medium. The chemical descriptors introduced and computed shall contribute to the foundation of the chemical reactivity on the conceptual and analytical physical bases, being able to predict the chemical transformations and the characterization of the bonds formation.

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