Abstract

Quantum theory of motion (QTM) is used to understand the Kolmogorov-Arnold-Moser (KAM) transition for Henon-Heiles oscillators. Conceptual density functional theory (CDFT) and its various allied global and local reactivity descriptors and the associated electronic structure principles are applied to rationalize the stability, reactivity and aromaticity of a variety of all-metal and non-metal systems. Different physico-chemical properties as well as toxicities of several aliphatic and aromatic electron acceptor and donor moieties are also analyzed under the structure-activity/structure-toxicity based protocol within the paradigm of the CDFT based reactivity descriptors.

The thesis is segregated into eight chapters. Chapter 1 provides an overall introduction and theoretical background used in the thesis. Chapter 2 contains the Kolmogorov-Arnold-Moser (KAM) transition from integrability to chaos in classical dynamical systems as mediated by the tuning of suitable parameters present in the Hamiltonian. For understanding the quantum signature of the classical chaos in this system a quantum theory of motion (QTM) has been made use of. Usefulness of various conceptual density functional theory (CDFT) based descriptors to analyze chemical reactivity when the atom is placed in confined environment as well as the prediction of acidity of meta/para substituted aromatic acids are discussed in chapter 3. A new DFT-based descriptor, Net electrophilicity ($\Delta\omega^{\pm}$) and its usefulness in analyzing the modes of different cycloaddition reactions as well as to construct valid quantitative structure activity relationship (QSAR)- based models for the toxicity of different halo-compounds is elaborated in chapter 4. In chapter 5, a DFT approach to investigate the stability, reactivity and aromaticity of two newly proposed super atoms, Al_7C^- and Al_7O^- and a super alkali-halogen cluster is elucidated. Chapters 6 and 7 delineate the stability, reactivity and aromaticity of different dianion clusters like Be_3^{2-}, Mg_3^{2-}, Ca_3^{2-} and their derivatives and the utility of trigonal cationic clusters like H_3^+, Li_3^+ and Na_3^+ to trap the noble gases as well as hydrogen in molecular and atomic forms respectively in the light of conceptual DFT. Chapter 8 elucidates the application of the number of carbon atoms (N_C) and the number of non-hydrogenic atoms (N_{NH}) to analyze different physico-chemical properties of alcohols, polychlorinated biphenyls (PCBs) etc as well as the toxicity of aliphatic and aromatic electron acceptors and donors towards the ciliated protozoa *Tetrahymena pyriformis*. Electrophilicity index (ω) and group philicity are used as additional descriptors.