Abstract

Density functional theory (DFT) can explain the behavior of a system in its ground state as well as in certain excited states. With the development of time dependent density functional theory (TDDFT) any time dependent quantity can be expressed as a functional of the charge density or probability density and the current density. An amalgamation of both the TDDFT and quantum fluid dynamics (QFD), leads to the quantum fluid density functional theory (QFDFT). In this theory the governing equation is a generalized nonlinear Schrödinger equation (GNLSE). The conceptual density functional theory has been successful in obtaining reactivity descriptors and associated electronic structure principles which can explain chemical reactivity and stability of a chemical system.

The thesis is segregated into seven chapters. Chapter 1 deals with the various theories used in understanding the reactivity and dynamics of confined atoms and molecules. Chapter 2 deals with the collision of confined atoms and molecules with protons. The interaction of atoms and molecules with an external electric field within a confined environment based on the dynamic profiles of chemical hardness, polarizability, chemical potential, entropy and electrophilicity index is presented in Chapter 3. In Chapter 4 the interaction of confined atom and molecule in ground as well as excited states with an external magnetic field is studied through the dynamic profiles of various reactivity parameters. Confinement of small gas molecules in BN cages and fullerene are studied in Chapters 5 and 6 respectively. The confinement induced binding of noble gas atoms is studied in Chapter 5. The probable existence of a chemical bond between noble gas (Ng) atoms has been analyzed. Chapter 6 deals with the confinement of atoms and molecules in fullerene cages. Chapter 7 presents a connection between the “classical” trajectories obtained from the trajectories generated using the “classical” wave function as it evolves according to the Newton’s equation of motion and compares it with the Bohmian trajectories obtained from the time dependent Schrödinger equation (TDSE) for a given system.