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An Overview of Quantum Chemistry and Molecular Dynamics

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Perspective

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ABSTRACT

Quantum chemistry, often known as molecular quantum mechanics, is a field of physical chemistry that studies how quantum mechanics might be applied to chemical processes. Quantum chemistry's core goal is to understand electronic structure and molecular dynamics by developing computer solutions to the Schrödinger equation.

INTRODUCTION

Chemists rely significantly on spectroscopy to gain information on the quantification of energy at the molecular level. Infrared spectroscopy (IR), Nuclear Magnetic Resonance (NMR) spectroscopy, and scanning probe microscopy are all common approaches. Quantum chemistry can be used to anticipate and verify spectroscopic as well as other types of experimental results.

The electronic ground state and excited states of individual atoms and molecules, as well as the study of reaction routes and transition states that occur during chemical processes, are the subject of many quantum chemistry investigations. It is also possible to predict spectroscopic properties. The electronic wave function is typically adiabatically parameterized by nuclear locations (i.e., the Born-Oppenheimer approximation) in such research. Semi-empirical methods, density functional theory, Hartree-Fock computations, quantum Monte Carlo methods, and coupled cluster methods are among the methods used.

The accuracy of results for small molecular systems is a major goal of quantum chemistry, as is the size of huge molecules that can be processed, which is limited by scaling considerations-computation time increases as a power of the number of atoms.

Some consider the discovery of the Schrödinger equation and its application to the hydrogen atom in 1926 to be the beginning of quantum chemistry. However, Walter Heitler (1904-1981) and Fritz London's article from 1927 is often regarded as the first milestone in the history of quantum chemistry. This is the first time quantum mechanics has been applied to the diatomic hydrogen molecule, and hence to the chemical bonding phenomenon. Robert S. Mulliken, Max Born, J. Robert Oppenheimer, Linus Pauling, Erich Hückel, Douglas Hartree, and Vladimir Fock, to name a few, made significant breakthroughs in the following years.

The 1838 discovery of cathode rays by Michael Faraday, Gustav Kirchhoff's 1859 statement of the black-body radiation problem, Ludwig Boltzmann's 1877 suggestion that the energy states of a physical system could be discrete, and Max Planck's 1900 quantum hypothesis that any energy radiating atomic system can theoretically be divided into a number of discrete energy elements such that each of these energy elements can theoretically be divided into a number of discrete energy elements.

Then, in 1905, Albert Einstein proposed, based on Planck's quantum hypothesis, that light itself consists of individual quantum particles, which later became known as photons, to explain the photoelectric effect (1839), i.e., that shining light on certain materials can function to eject electrons from the material (1926). This theoretical foundation was gradually applied to chemical structure, reactivity, and bonding in the years that followed. Linus Pauling made the most significant contribution to the field.

Electronic structure

Electronic structure is the focus of this study. Solving the Schrödinger equation (or Dirac equation in relativistic quantum chemistry) with the electronic molecule Hamiltonian is usually the initial step in solving a quantum chemical problem.

This is known as determining the molecule's electronic structure. It can be claimed that a molecule's or crystals electrical structure fundamentally reflects its chemical properties. Only the hydrogen atom provides a precise solution to the Schrödinger equation (though exact solutions for the bound state energies of the hydrogen molecular ion have been identified in terms of the generalized Lambert W function). Because the motions of three or more "particles" are involved in every other atomic or molecular system, the Schrödinger equations can't be solved accurately, hence approximate solutions must be sought.

Bond of valence

Theory of Valence Bonds is the main article. Although Schrödinger established the mathematical foundations of quantum chemistry in 1926, it is widely acknowledged that the first authentic quantum chemistry calculation was