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Short Communication

Advances in Inorganic Chemistry

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DESCRIPTION

Chemical bonding, chemical reaction, valence, the surface of potential energy, molecular orbitals, orbital interactions, and molecule activation are examples of theoretical generalisations developed by theoretical chemistry. Theoretical chemistry brings together principles and concepts that are present in all fields of chemistry. The systematization of chemical laws, principles, and norms, as well as their refining and detailing, and the development of a hierarchy, are all part of theoretical chemistry. The theory of the connectivity of the structure and properties of molecular systems is at the heart of theoretical chemistry. It employs mathematical and scientific approaches to describe the structures and dynamics of chemical systems, as well as to correlate, comprehend, and forecast their thermodynamic and kinetic properties. In the broadest sense, it is the use of theoretical physics approaches to explain chemical processes. Unlike theoretical physics, theoretical chemistry frequently employs semi-empirical and empirical methodologies in conjunction with the tremendous complexity of chemical systems. Quantum chemistry is the application of quantum mechanics to chemistry problems, has dominated the field in recent years. Molecular dynamics, statistical thermodynamics, electrolyte solution theories, reaction networks, polymerization, catalysis, molecular magnetism, and spectroscopy are some of the other significant components.

In current theoretical chemistry, the study of chemical structure and the study of chemical dynamics are largely separated. Electronic structure, potential energy surfaces, and force fields; vibrational-rotational motion; and equilibrium features of condensed-phase systems and macromolecules are examples of the former. Bimolecular kinetics and the collision theory of reactions and energy transfer are examples of chemical dynamics, as are unimolecular rate theory and metastable states, as well as condensed-phase and macromolecular elements of dynamics.

Various branches in theoretical chemistry

Quantum chemistry: Quantum mechanics or fundamental interactions are used to chemical and physico-chemical problems. The most commonly modelled properties are spectroscopic and magnetic.

Computational chemistry: Computation systems such as Hartree–Fock,post–Hartree–Fock,density functional theory, semiempirical methods (such as PM3), and force field methods are used in the application of scientific computing to chemistry. The most commonly anticipated attribute is the form of the molecules. Computers can also acquire and Fourier transform Infrared Data into frequency information, as well as forecast vibrational spectra and vibronic coupling. The projected form is supported by a comparison to predicted vibrations.

Molecular modelling: Methods for simulating molecular structures that do not require the use of quantum mechanics. Molecular docking, protein-protein docking, drug design, and combinatorial chemistry are some examples.

Molecular dynamics: Simulating the movement of the nuclei of an assembly of atoms and molecules using classical mechanics. Van der Waals forces govern and temperature stimulate the rearrangement of molecules within an ensemble.

Molecular mechanics: Potentials are used to model the intramolecular and intermolecular interactions' potential energy surfaces. Ab initio calculations are commonly used to parameterize the latter.

Mathematical chemistry: Mathematical methods are used to discuss and predict the molecular structure without referring to quantum mechanics. Topology is an area of mathematics that helps scientists to predict the properties of flexible finite-size bodies such as clusters.

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Theoretical chemical kinetics: Theoretical investigation of the dynamical systems associated with reactive chemicals, activated complexes, and the differential equations that govern them.

Cheminformatics: The application of computer and informational tools to agricultural data in the field of chemistry to address difficulties.

Chemical engineering: To undertake research and development, chemistry is used to industrial processes. This enables the creation and refinement of new and existing goods as well as industrial processes.