Computational Chemistry:

The first theoretical calculations in chemistry were those of Walter Hitler and Fritz London in 1927. The books that were influential in the early development of computational quantum chemistry include Linus Pauling and E. Bright Wilson's 1935 Introduction to Quantum Mechanics – with Applications to Chemistry, Heitler's 1945
In the early 1950s, the first semi-empirical atomic orbital calculations were performed. Theoretical chemists became extensive users of the early digital computers. One major advance came with the 1951 paper in Reviews of Modern Physics by Clemens, largely on the "LCAO MO" approach (Linear Combination of Atomic Orbitals Molecular Orbitals), A very detailed account of such use in the United Kingdom is given by Smith and Sutcliffe. The first ab initio Hartree–Fock method calculations on diatomic molecules were performed in 1956, using a basis set of Slater orbitals. For diatomic molecules, a systematic study using a minimum basis set and the first calculation with a larger basis set were published in 1960
In 1964, Hückel method calculations (using a simple linear combination of atomic orbitals (LCAO) method to determine electron energies of molecular orbitals of π electrons in conjugated hydrocarbon systems) of molecules, ranging in complexity from butadiene and benzene . These empirical methods were replaced in the 1960.

One of the first mentions of the term computational chemistry can be found in the 1970 book Computers and Their Role in the Physical Sciences, widely different methods began to be seen as part of a new emerging discipline of computational chemistry. The Journal of Computational Chemistry was first published in 1980.

Computational chemistry has featured in several Nobel Prize awards, most notably in 1998 and 2013.
Computational chemistry is a branch of chemistry that uses computer simulation to assist in solving chemical problems. It uses methods of theoretical chemistry, incorporated into efficient computer programs, to calculate the structures and properties of molecules .

Examples of such properties are structure, absolute and relative (interaction) energies, electronic charge density distributions, dipoles and higher multipole moments, vibrational frequencies, reactivity, or other spectroscopic quantities.

Computational chemistry is a new discipline. Its advent and popularity have paralleled improvements in computing power during
the last several decades ,and uses tools to understand chemical reactions and processes.
computational chemistry are to characterize and predict the structure and stability of chemical systems, to estimate energy differences between different states,

Fields of application

The term *theoretical chemistry* may be defined as a mathematical description of chemistry, whereas *computational chemistry* is usually used when a mathematical method is sufficiently well developed that it can be automated for implementation on a computer. In theoretical chemistry, chemists, physicists, and mathematicians develop algorithms and computer programs to predict atomic and molecular properties and reaction paths for chemical reactions.

Computational chemistry has two different aspects:

- Computational studies, used to find a starting point for a laboratory synthesis, or to assist in understanding experimental data, such as the position and source of spectroscopic peaks.
- Computational studies, used to predict the possibility of so far entirely unknown molecules or to explore reaction mechanisms not readily studied via experiments.

Several major areas may be distinguished within computational chemistry:

- The prediction of the molecular structure of molecules by the use of the simulation of forces, or more accurate quantum chemical methods, to find stationary points on the energy surface as the position of the nuclei is varied.
- Storing and searching for data on chemical entities (see chemical databases).
- Identifying correlations between chemical structures and properties (see *quantitative structure–property relationship* (QSPR) and *quantitative structure–activity relationship* (QSAR)).
- Computational approaches to design molecules that interact in specific ways with other molecules (e.g. drug design and catalysis).

Accuracy

Computational chemists often attempt to solve the non-relativistic Schrödinger equation, although some progress has been made in solving the fully relativistic Dirac equation. In principle, it is possible to solve the Schrödinger equation in either its time-dependent or time-independent form, as appropriate for the problem in hand; in practice, this is not possible except for very small systems. Therefore, a great number of approximate methods strive to achieve the best trade-off between accuracy and computational cost.

Accuracy can always be improved with greater computational cost.

This complicates the study of molecules interacting with high atomic mass unit atoms, such as transitional metals and their catalytic properties. Present algorithms in computational chemistry can routinely calculate the properties of small molecules that contain up to about 40 electrons.

Large molecules can be studied by semi-empirical approximate methods. Even larger molecules are treated by classical mechanics methods that use what are called molecular mechanics (MM). In QM-MM methods, small parts of large complexes are treated quantum mechanically (QM),And the remainder is treated approximately (MM).

Branches of theoretical chemistry

Quantum chemistry

> The application of quantum mechanics or fundamental interactions to chemical and physico-chemical problems.

Computational chemistry

> The application of computer codes to chemistry, involving approximation schemes such as Hartree–Fock, density functional theory, semiempirical methods (such as PM3) or force field methods. Computers can also predict vibrational spectra

Molecular modelling

Methods for modelling molecular structures without necessarily referring to quantum mechanics. Examples are molecular docking, protein-protein docking, drug design, combinatorial chemistry.

Molecular mechanics

Modeling of the intra- and inter-molecular interaction potential energy surfaces via potentials. The latter are usually parameterized from ab initio calculations.

Theoretical chemical kinetics

Theoretical study of the dynamical systems associated to reactive chemicals, the activated complex and their corresponding differential equations.

cheminformatics

The use of computer and informational techniques, applied to crop information to solve problems in the field of chemistry.

The types of predictions possible for molecules and reactions include

1-Heats of formation

2-bond and reaction energies

3-Molecular energies and structures (thermochemical stability)

4-Energies and structures of transition states (activation energies)

5-charge distribution in molecules (reactive sites)

6-vibrational frequencies (IR and Raman spectra)

Electronic transition (UV/ Visible spectra)

7-Magnetic shielding effects (NMR spectra).

Prediction of these properties has many applications in energetic materials research , including studies of synthesis pathways , reaction products , and initiation mechanisms.