

Role of chemistry in computer science & engineering

Lecture – 3

Department of CSE, DIU

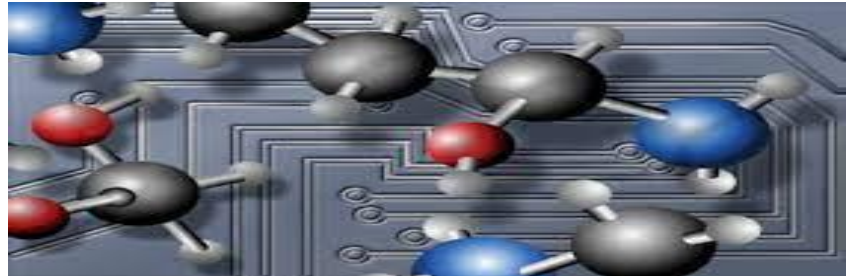


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Uses and effects of chemistry



Computational chemistry uses result of theoretical chemistry incorporated into efficient computer programmed to calculate structure and properties of molecule.

It calculate the properties of molecule such as structure, relative energy, charge distribution, dipole moment, vibrational frequency, reactivity and other spectroscopic quantity.

Computational chemistry range from highly accurate (Ab initio method to less accurate (semiempirical) to very approximate (molecular mechanics).

(ab initio and semiempirical will be discussed later)*

Cont.

In the past two decades, computational molecular modeling approaches (Leach, 2001) have emerged as important tools that **can be used to predict atomic structure, vibrational frequencies, binding energies, heats of reaction, electrical properties, and mechanical properties of organic and inorganic materials.**

Benefits of Chemistry

- 1) It allows the medicinal chemist for use the computational power of computer for measurement of Mol. geometry electron density electrostatic potential conformational analysis different types of energies.
- 2) Determination of structure of ligand and target through X-ray crystallography and NMR spectroscopy.
- 3) Docking of ligand in receptor active sites and exact measurement of geometric and energetic favor ability of such interaction.
- 4) Comparssion of various ligands throgth various parameters.

Relation Between Chemistry and Computer Science



Applications of Chemistry

https://en.wikipedia.org/wiki/Computational_chemistry



- 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.

Thus, computational chemistry can assist the experimental chemist or it can challenge the experimental chemist to find entirely new chemical objects.

- [is](#)).

Cont.

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 Identifying correlation between chemical structure and properties .
- Computational approaches to help in the efficient synthesis of compounds.
- Computational approaches to design molecules that interact in specific ways with other molecules(e.g. Drug design and catalysis)

Watch:

<https://www.youtube.com/watch?v=MA9pnR6VvBw>

**Thank
You**

