

## Lecture 1.3 & 2.1

### Role of chemistry in computer science & engineering

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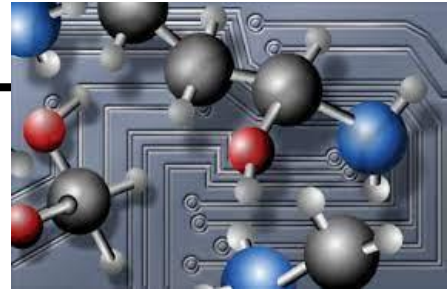
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# Uses and effects of chemistry



**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 (**Semi empirical method** ) to very approximate (molecular mechanics).  
(ab initio and semi-empirical will be discussed later)\*

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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.**

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# Benefits of Computational Chemistry

- 1) It allows the medicinal chemist to use the computational power of computer for measurement of Mol. geometry , electron density , electrostatic potential, conformation analysis , different types of energies etc ...
- 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 favorability of such interaction.
- 4) Comparison of various ligands through various parameters.

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# Applications of Computational Chemistry

[https://en.wikipedia.org/wiki/Computational\\_chemistry](https://en.wikipedia.org/wiki/Computational_chemistry)

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- 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.

- 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 nuclear is varied.
- 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**

