ENGINEERING CHEMISTRY

Department of Science and Humanities

ENGINEERING CHEMISTRY

Module I- COMPUTATIONAL CHEMISTRY

- INTRODUCTION
- COMPUTATIONAL METHODS
- APPLICATIONS

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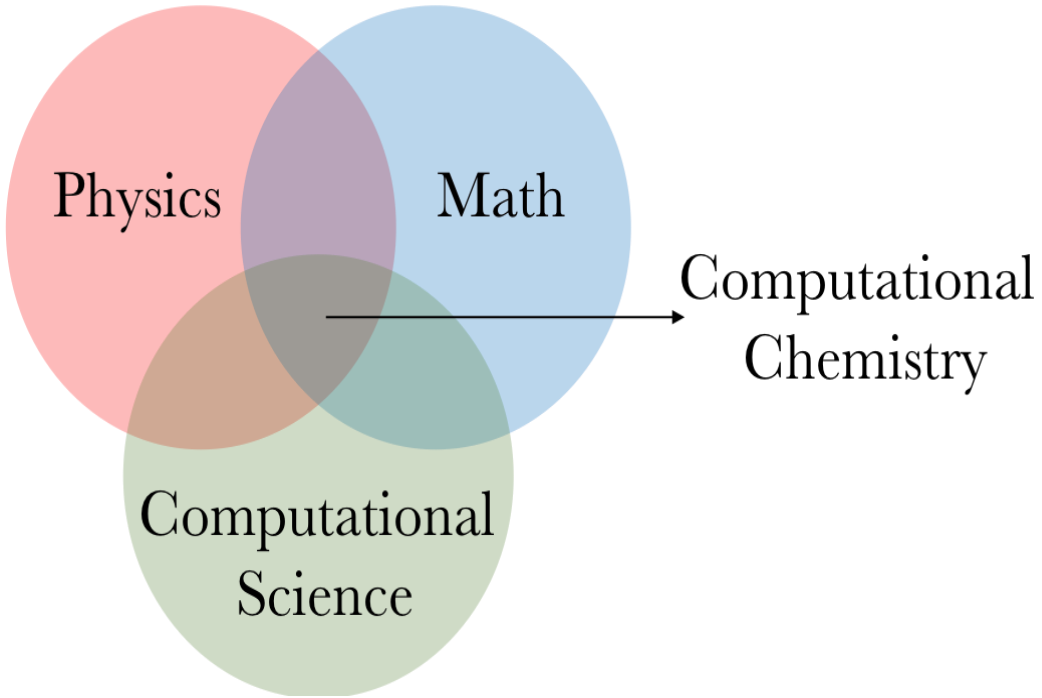

Introduction

Computational chemistry is a set of techniques for the investigating chemical problems on a computer rather than using chemicals.

It uses the results of theoretical chemistry incorporated into efficient computer programs to calculate the properties of a molecule.

The first theoretical investigation was done by Walter Heitler and Fritz London in 1927

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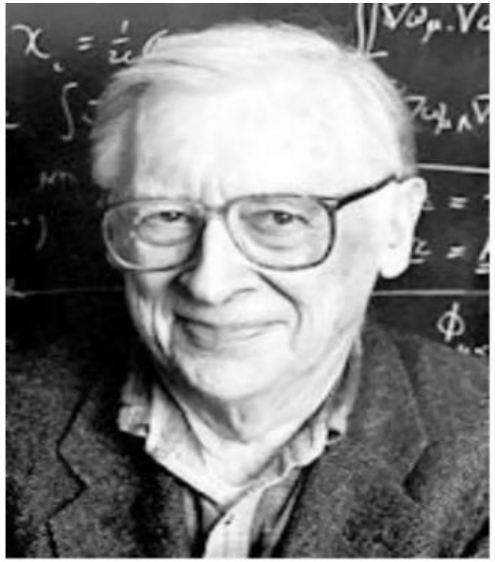
Walter Kohn



John A. Pople

1998

Walter Kohn : For the development of density functional theory.

John A. Pople : For the development of computational methods in quantum chemistry.

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2013

For the development of computer based methods to model complex systems.

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Objective of computational chemistry:

To solve chemistry problems by simulating chemical systems (molecular, biological, materials) to provide reliable, accurate and comprehensive information at an atomic level.

Advantages of computational chemistry:

- Calculations are easy to perform than carrying experiments.
- Calculations are less costly, whereas experiments are becoming more expensive
- Calculations are safe than performing experiments.

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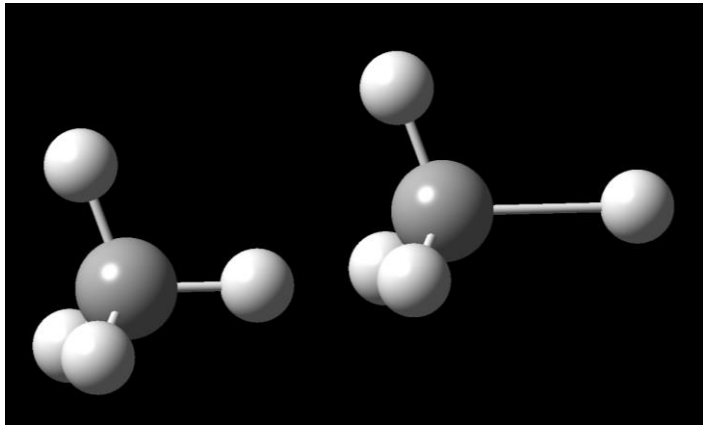
Scope of computational modeling:

Molecular Properties:



Computational modeling can be used to accurately predict the physical and chemical properties of molecules, such as

- Bond lengths, Bond angles and HOMO/LUMO
- Can predict the spectra of UV-Vis, IR and NMR
- Thermodynamic and kinetic properties
- Electronic structure and mechanical properties

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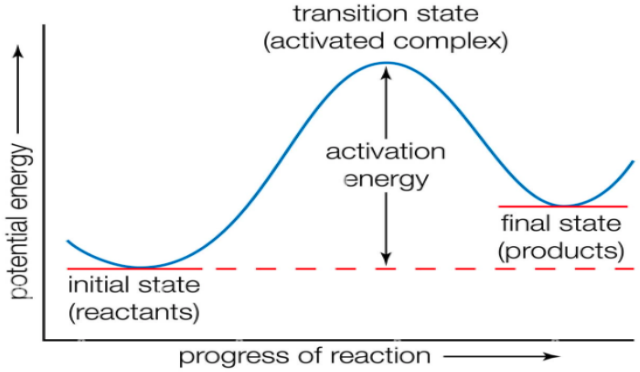
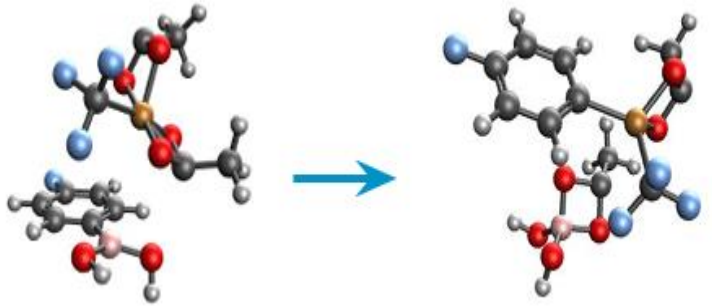
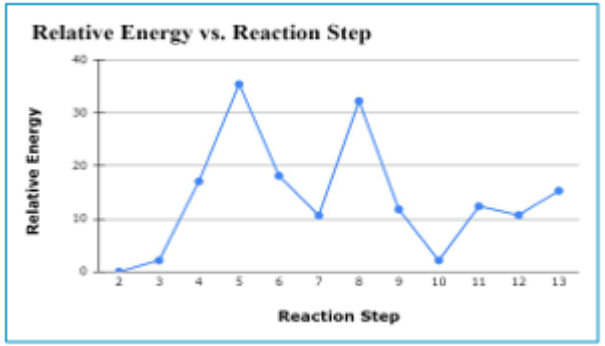
Reaction mechanism:

To know the underlying reaction mechanism and the kinetics of a reaction mechanism computational chemistry plays a vital role.







Material design:

Computational modeling enables the rational design of new materials with desired properties such as high electrical conductivity, thermal stability etc. This leads to the development of advanced materials for energy production and storage applications, electronics and much more.

Ref: Computational Analysis of Reaction Mechanism for Trifluoromethylation of Organic Compounds

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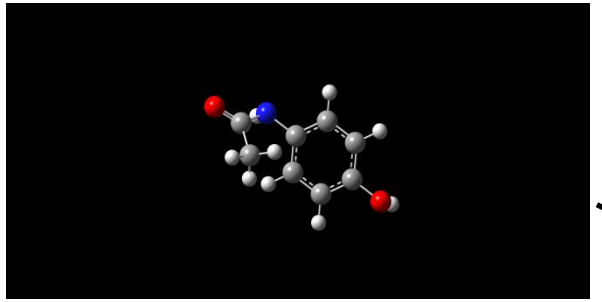
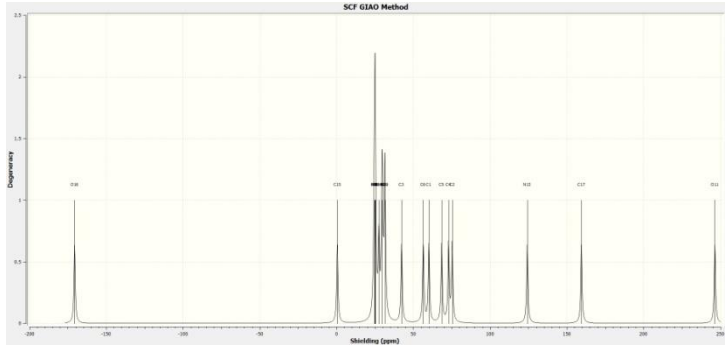
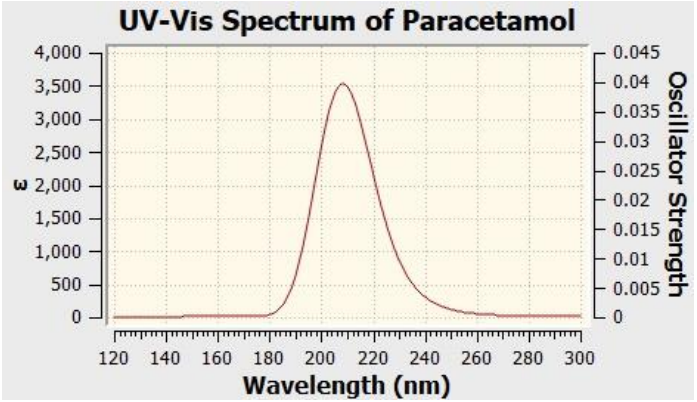
Drug discovery:

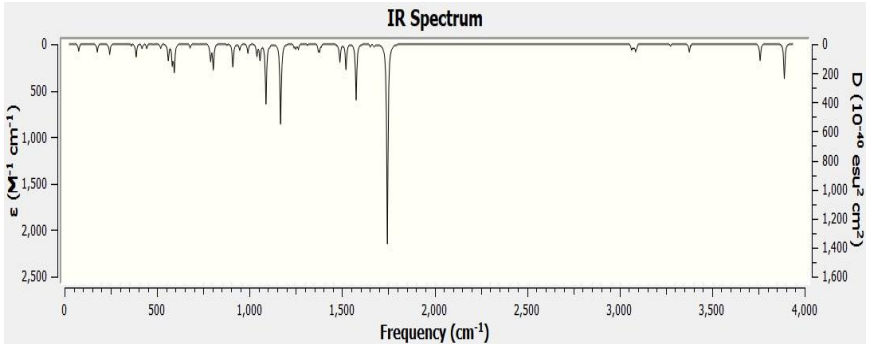
Computational chemistry plays a pivotal role in design and screening of potential drug candidates by simulating the interactions between the drug molecules and biological targets.



Paracetamol







All these spectra are generated using Gaussion 16

THANK YOU

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