ENGINEERING CHEMISTRY

PES UNIVERSITY
CELEBRATING 50 YEARS

Department of Science and Humanities

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Module I- COMPUTATIONAL CHEMISTRY

Computational methods:

There are two main methods depending on the starting point theory:

Classical method:	Quantum chemistry method :
• These use Newton mechanics to model molecular system. • Atom – Sphere, Bonds – Springs and Electrons are ignored. • Total potential energy of a molecule is given by sum of all the energies of attractive and repulsive forces between atom in structure.	• These use quantum mechanics to model the molecular system. • It is based on arrangement of electrons in molecules and interaction of these electrons with electron and nuclei of another molecule. • We consider that electron and all other particle exhibits both particle and wave nature.
i. Molecular mechanics ii. Molecular dynamics	i. Semi empirical methods. ii. Ab initio methods iii. Density functional theory

Ref. Book: Introduction to computational chemistry by Frank Jensen, Wiley publications

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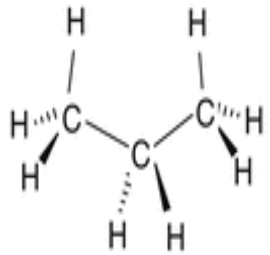
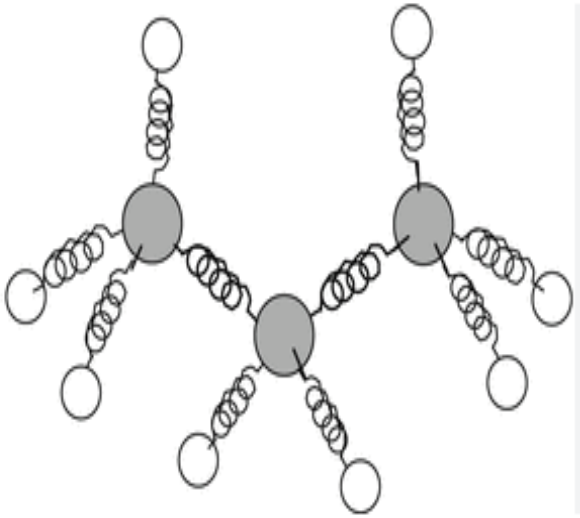
Molecular mechanics:

- Molecular mechanics programs use equations based on classical physics to calculate force fields.
- It is based on the model of a molecule as a collection of balls(atoms) held together by springs(bonds).
- Its too fast like a very large molecules like steroids can be optimized in seconds and allows geometry optimization .





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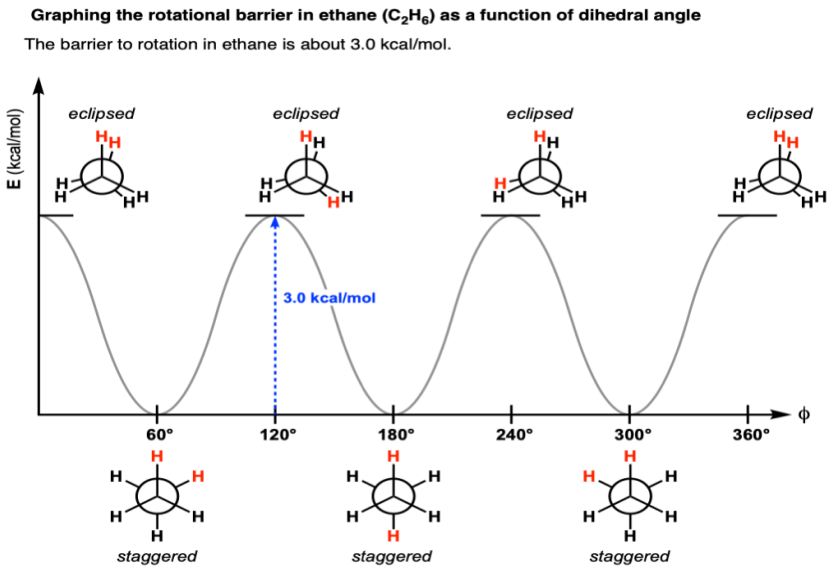
Molecular dynamics:

- Molecular dynamics is a molecular mechanics program designed to mimic the movement of atoms within a molecule. The laws of motion to molecule is the base for it.
- Molecular dynamics can be carried out on a molecule to generate different conformation which on energy minimization.



Staggered vs Eclipsed Conformations of Ethane - Master Organic Chem

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Semi empirical methods:

- Semi empirical calculations are based on Schrödinger equation.
- It represents a middle road between the mostly qualitative results available from molecular mechanics and the high computationally demanding quantitative results from Ab initio methods.
- Capable of calculating transition states and excited states.

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Ab initio calculations:

- Ab initio calculations are based on Schrödinger equation and it describes, among other things, how the electrons in a molecule behave.

- The wave function is a mathematical function that can be used to calculate the electrons distribution.

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Density functional theory

- DFT are like Ab initio and semi empirical calculations, based on Schrödinger equation.
- However, unlike the other two methods, DFT does not calculate a conventional wave function, but rather derives the electron distribution directly.
- Density functional calculations are usually faster than Ab initio, but slower than semi empirical method.

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Applications of computational chemistry

- Electronic structure predictions and energy minimizations.
- Finding transition structure and reaction paths and molecular docking: protein – protein, protein – ligand interactions.
- Thermochemistry : heat of reactions, energy of activation, etc.
- Calculation of many other molecular, physical and chemical properties.

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Conclusion:

- Computational chemistry plays a pivotal role in advancing our understanding of chemical systems and accelerating scientific discovery.

- Its advantages in cost-effectiveness, efficiency, safety, accessibility, versatility, and accuracy make it an indispensable tool in modern research and development.

- Computational chemistry is not a replacement for experimental studies, but plays an important role in enabling chemists to design and develop the desired chemicals/ products.

Ref. Book: Introduction to computational chemistry by Frank Jensen, Wiley publications

THANK YOU

Department of Science and Humanities