Lecture 1: Introduction

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Chem 150/250 Fall 2022
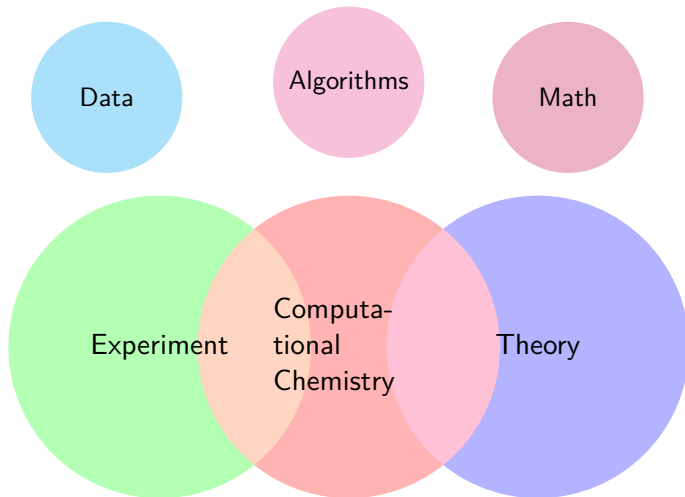
09/29/2023

What Is Computational Chemistry?

What is a Theory?

- Theories are sets of logical statements, and in science they are often expressed by equations.
- Theories are not data
- Scientific theories explain on empirical observation. However, most powerful theories require only minimal empirical input (e.g. natural constants)
- Chemical theories make statements about chemical observables, such as molecular energetics, properties, kinetics, reactivity, mechanisms, etc.
- Examples: Phlogiston theory, Chemical thermodynamics, Ligand field theory

Axioms

- Essence of a theory: set of axioms or "first principles"
- In scientific theories are statements about measurable quantities, or the conditions of measurability.
- Axioms must be
    - as simple as possible (parsimony)
    - as general as possible
    - as accurate as possible
    - as few as possible
- Examples: Postulates of quantum mechanics

What Is an Experiment?

- Scientific experiments are theory-guided observations of natural phenomena that
  - are controlled and reproducible, independent of individual,
  - yield a unique result,
  - answer a well-posed (theoretical) question.
- Experiments are never wrong, but can be poorly executed.
- Examples of chemical experiments: reactivity studies, total synthesis, characterization etc.

Theory-Ladenness of Observation[1]

[1] Hanson72.