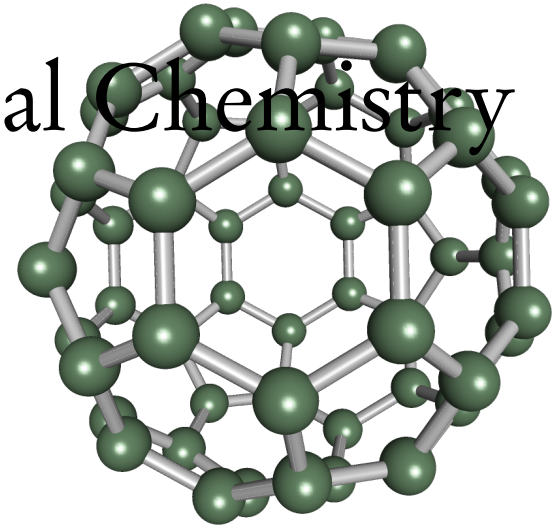
Theoretical and Computational Chemistry
Lecture 1

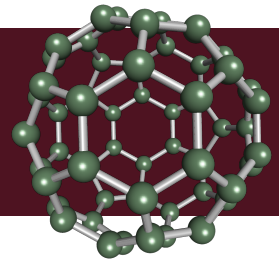


CHEM203 — Physical Chemistry

☎ 04 463 6760 (internal ext. 6760)

Alan MacDiarmid Bldg. 2nd Floor, Office 203

Housekeeping



- Lecture slides, practise questions and assignment are available on BlackBoard
- Assignments: Due date as on BlackBoard (Online submission only)
- Computational Chemistry Tutorials in **KK216 Cyber Comms**
  Will be focussed on the assignment, which is a computer lab
  Should take approximately 2 - 3 hours (in total) to complete
  Thursdays and Fridays from 9 am 10 am (weeks beginning 30 Sept and 7 Oct)

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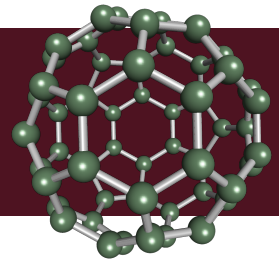
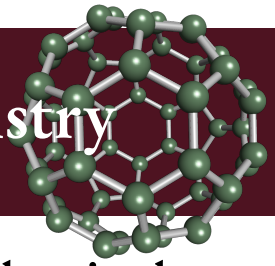


Apart from Atkins & de Paula Physical Chemistry 9th ed, Oxford

Jensen Introduction to Computational Chemistry 2nd ed, Wiley
Cramer Essentials of Computational Chemistry 2nd ed, Wiley
Lewars Computational Chemistry, 2nd ed, Springer

Theoretical and Computational Chemistry



All Computational Chemistry is built upon some form of physical description of a molecular system

Definition

Sometimes this description uses fundamental physical concepts and builds everything from scratch (***ab-initio***)

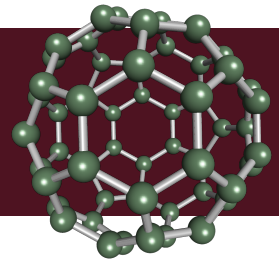
Definition

Sometimes a mixture between fundamental concepts and some empirical parameters is used (***semi-empirical***)

Definition

Sometimes the description is purely phenomenological and our description is based on a loose analogy with a different system (***empirical***)

Ab-Initio Methods



The domain of physics that describes how electrons and protons interact is Quantum Mechanics[1]
Models that solve the **Schrödinger Equation** are called "**ab-initio**" (from the beginning). This is the realm of Quantum Chemistry.

$$\hat{H}\Psi(\tau) = \mathcal{E}\Psi(\tau)$$

$$\hat{H} = \sum_{a=1}^{M}\sum_{b<a}^{M}\frac{Z_a \cdot Z_b}{r_{ab}} - \sum_{i=1}^{N}\sum_{a=1}^{M}\frac{Z_a}{r_{ia}} + \sum_{i=1}^{N}\sum_{j<i}^{N}\frac{1}{r_{ij}} - \sum_{i=1}^{N}\frac{1}{2}\nabla_i^2 - \sum_{a=1}^{M}\frac{1}{2m_a}\nabla_a^2$$

[1](Note: There is more than one Quantum Theory and some problems in Chemistry require us to go beyond the Schrödinger Equation. For example the Dirac Equation for systems with heavy atoms to include the effects of Special Relativity Theory or Quantum Electrodynamics for highly accurate descriptions)