

2H43 THEORETICAL CHEMISTRY

Atomic structure

6 Lectures/workshops by Dr S. H. Ashworth.

Material

The Bohr model: How good is the classical approach to the hydrogen atom?

The hydrogen atom: An exact solution of the Schrödinger equation for an atomic system.

One electron orbitals: The shapes and extents of the orbitals produces as solutions for the H atom.

The helium atom: An approximate solution of the Schrödinger equation.

The Pauli exclusion principle: How this arises and its implications

The variational principle: How we know an approximate solution is never lower than reality.

Objectives

After completing this part of the course you should be able to demonstrate that you can:

- Derive the Bohr model of the H atom.
- Describe how to solve the Schrödinger equation for the H atom.
- Describe how quantum numbers and their bounding values arise in the solutions.
- Draw H atom orbitals: both radial and angular parts.
- Describe approximations involved in the solution of the Schrödinger equation for the helium atom.
- Describe electron-electron pair effects.
- Write down the Pauli principle and explain how it arises.
- Describe the variational principle and how it may be used in calculations.
- Use angular momentum operators and commutator algebra in simple problems.