National Training School in Theoretical Chemistry

Electronic structure theory

Fred Manby (Bristol), 4 lectures plus tutorial

In electronic structure theory, the assumption of the Born-Oppenheimer approximation has been made, and the remaining problem concerns the accurate, but inevitably approximate, solution of the electronic Schrödinger equation.

In these lectures we will first study how this can be done in the mean-field approximation, ie through Hartree-Fock theory. The discussion will be necessarily brief, but we will certainly make sure that there is time to discuss some of the interesting features of this fundamental theory.

In the second lecture, we will explore one of the key tools of modern computational chemistry: density functional theory (DFT). I will cover the fundamental basis of DFT; Kohn-Sham theory as a means of *doing* DFT; and the development of approximate exchange-correlation functionals.

The remainder of the course will be dedicated to the issue of electron correlation, with a focus on dynamic correlation and single-reference electronic structure theory. In particular we will see how another fundamental pillar of quantum mechanics — perturbation theory — can help us, and also explore the more advanced topics of configuration interaction and coupled cluster theory.

The course will build on the quantum mechanics lectures by Prof Knowles, given earlier in the Summer school.