National Training School in Theoretical Chemistry

Liquid State Theory

George Jackson (Imperial College London), 3 lectures, 1 problem class

A molecular description of matter using statistical mechanical theories and computer simulation is the key to understanding and predicting the properties of dense fluids and materials. Fluid systems form an integral part of our modern lifestyle from the use of simple solvents in chemical processing to the design of opto-electronic devices with liquid crystalline and polymeric materials.

As well as being of inherent scientific interest, the link between the microscopic interactions between small numbers of molecules and the macroscopic properties of the bulk system comprising them is of great industrial relevance.

In this part of the course the main theoretical achievements in liquid state theory will be outlined. This with range from the original approach of van der Waals (1973), through the use of correlation functions to describe the properties of fluids (1950s-1980s), to the more sophisticated density functional theories of inhomogeneous fluids (1980s-date). The most recent developments in statistical mechanical theories which are used to probe the bulk or interfacial properties of fluids will be reviewed making contact with the description of real systems wherever possible. The focus will be on the structural and thermodynamic properties, with an emphasis on phase equilibria.