

Theoretical and Computational Developments for Next Generation Thermodynamic Modelling of Complex Fluids

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The fundamental phase diagram of a pure substance exhibiting gas, liquid and solid phases is reasonably well understood. As the pioneering work of van der Waals showed, the fluid phase behaviour of 'simple' fluids can be understood in terms of the balance of spherical repulsive and attractive forces, and even the fluid-solid transition of such systems can be explained in terms of the freezing of a hard-sphere system. A challenge, however, arises when trying to describe, and even predict, accurately the properties of a given substance or mixture of substances. Modern equations of state, such as SAFT (statistical associating fluid theory), which are based on detailed molecular models have greatly enhanced the capability of analytical methods and provide a tool that can be used to study complex fluids. I will discuss some of the recent advances in this area; especially the recasting of the free energy expression into a group contribution method and the advantage of incorporation of generalised Lennard-Jonesium potentials. With this framework in place, the analytical approach (the equation of state) can be used to develop so-called force-fields for use in computer simulation. The importance of taking a molecular perspective towards complex systems is highlighted as the design of novel materials is guided by a theoretical understanding.