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Internal Seminar

Theory for Freezing Transition: Density Functional Approach

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A free energy functional for a crystal that contains both the symmetry conserved and symmetry broken parts of the direct pair correlation function has been used to investigate the crystallization of fluids in three-dimensions. The symmetry broken part of the direct pair correlation function has been calculated using a series in ascending powers of the order parameters and which contains three- and higher-bodies direct correlation functions of the isotropic phase. It is found that a very accurate description of freezing transitions for a wide class of potentials is found by considering the first two terms of this series. We have investigated fluid-crystal transition using this theory for hard spheres, Inverse power potentials, purely repulsive WCA Lennard - Jones (RLJ) potential, the full Lennard - Jones (LJ) potential and square shoulder potentials fluids. The results found for freezing parameters for the fluid - face centred cubic (fcc) crystal transition are in very good agreement with simulation results. In Inverse power potential fluids, it is found that for $n > 6.5$ the fluid freezes into fcc structure while for $n \leq 6$ it freezes into base centred cubic (bcc) structure. The fluid-bcc-fcc triple point is found at $(1/n) = 0.158$ which is also in very good agreement with simulation value. In this theory, it is shown that although the contribution made by the symmetry broken part to the grand thermodynamic potential at the freezing point is small compared to that of the symmetry conserving part, its role is crucial in stabilizing the crystalline structure and on values of the freezing parameters.

Monday, Oct 24th 2016

2:00 PM (Tea/Coffee at 1:45 PM)

Seminar Hall, TCIS