The Open University

School of Mathematics & Statistics

Applied Mathematics Colloquium

Statistical Mechanics of Classical Fluids: Density Functional Theory and Equilibrium and Dynamics of Wetting

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15:30
Room 306 Alan Turing

Abstract:

In this talk we will demonstrate the apparatus of the classical density functional theory (DFT), which is a valuable computational statistical-mechanical framework to analyze fluids at the nano-scale, where the fluid inhomogeneity and the non-locality of the intermolecular interactions can lead to complicated spatial dependences of the fluid density. Taking the fluid inhomogeneity into account is important in problems dealing with phase transformations, interfaces and kinetics of soft systems. As part of this talk, we will discuss novel, first-order and continuous, interfacial transitions, including wetting, pre-wetting, capillary-condensation and filling, the formation of nanodroplets and liquid bridges, which can occur in sculpted pores with one or more dimensions on the order of several nanometers. These transitions are sensitive to both the range of the intermolecular forces and the interfacial fluctuation effects. We will show how DFT allows one to systematically obtain the thermodynamic phase portrait of a soft-matter system, including the regions of metastability of the different configurations.

Within DFT, the grand free energy of a classical soft-matter system is expressed as a functional of the system's one-body density field. Therefore, equilibrium DFT can be viewed as a method to introduce the spatial dependence of the fluid density into the thermodynamic equation of state. The dynamic DFT (DDFT) in its simplest form is a generalized diffusion equation corresponding to the Smoluchowsky picture of the dynamics of colloidal particles in a solvent. The DDFT can capture diffusion driven evolution of soft matter systems, while keeping track of atomic scale changes in the fluid structure. We will show how DDFT can yield a picture of diffusion-driven spreading and coalescence of sessile nanodroplets. We hope to demonstrate that (D)DFT is capable of bridging the gap between purely atomistic [e.g., Molecular Dynamics simulations] and continuum mechanical [e.g., Navier–Stokes (NS)] descriptions of soft condensed matter, while retaining essential microscopic details of large systems at a computational cost significantly lower than MD.

Tea and coffee will be available in the common area from 15:00