

Chemical Engineering Graduate Seminar



Dr. Athanassios Z. Panagiotopoulos
Princeton University

3:30 – 4:30 PM

April 27, 2004

CPE 2.218

“Molecular And Mesoscopic Simulations Of Phase Equilibria”

This presentation summarizes recent work on modeling phase transitions in ionic, surfactant and colloid/polymer systems. The unifying characteristic of these complex fluids is the close interplay between microstructure and macroscopic properties and the existence of strong interactions or multiple relevant length and time scales. Two complementary approaches are used to render the computational problem tractable, namely drastic simplification of the model studied to retain only essential physical characteristics and development of powerful Monte Carlo sampling methodologies to avoid getting trapped in local free energy minima and to cover large regions of parameter space in an efficient way. Ongoing investigations of phase transitions in systems under shear will also be described.