16:155:513 **Fundamentals of Nanoscale Thermodynamics and Transport**

Syllabus. Nanoscale science and engineering operates with physical, chemical, and biological processes and objects, in which at least one dimension is smaller than micron. At the same time, the details of molecular structure and inter-molecular interactions are left to the domain of quantum mechanics. The nanoscale spans the range from ~ 1 nm (10 A) to ~1000 nm (1 mkm). The course covers the theoretical and multiscale simulation methods, which bridge macroscopic thermodynamics and continuum transport theories with atomistic quantum mechanics and molecular dynamics. The key theoretical topics include: statistical mechanics and thermodynamics of nanophases and nanostructured materials, Monte Carlo simulation of nanoscale systems, density functional theory of confined fluids, coarse-grained molecular dynamics and dissipative particle dynamics. The applications include: nanoparticles and nanocomposites, porous materials, nanostructured colloids and surfaces, self-assembled surfactant and polymeric systems, lipid bilayers and cell membranes. This class is designed for PhD and MS chemical engineering students with interest in theoretical modeling and computations. The students will get experience with modern molecular and mesoscale simulation tools by performorming two computational term projects.

Pre-requisites: basic chemical engineering classes on thermodynamics and transport, good computer skills, knowledge of at least one programming language (any language: Fortran, C, Python, MATLAB, etc). A qualifying homework will be given at the 1st session to check student preparation for the class.
Computer requirements: Rutgers NET ID and a personal computer with installed Fortran compiler to run the programs used in the class. Instructions on installation will be provided.
Recommended book: D. Frenkel and B. Smit, Understanding molecular simulations, 2nd Edition, 2001