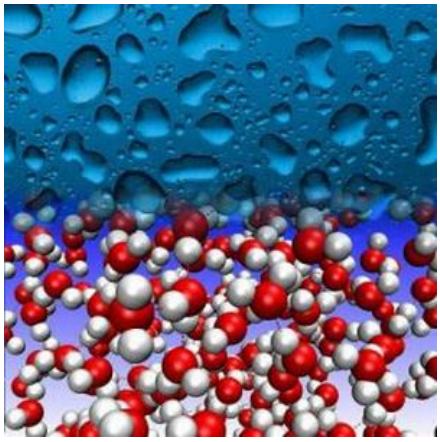
ChE 702: ST "Statistical Thermodynamics and Molecular Modeling"

for graduate students in ChemE, Physics, MechE, Chemistry

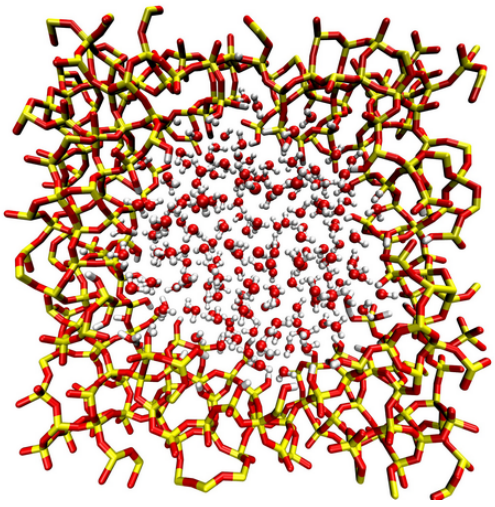
Instructor: Prof. Gennady Gor gor@njit.edu
http://chemicaleng.njit.edu/people/gor.php
Semester: Spring 2017
Hours: Thursdays, 6:00-9:05 PM



Today molecular simulations became a significant complement to "paper-and-pencil" theory and experimental research. Moreover, often molecular simulations can substitute experimental research being much cheaper, safer and faster. Molecular simulations are used in numerous various fields, e.g. they are applied to study problems related to drug design, protein folding and aggregation; wetting phenomena and hydration thermodynamics; nucleation and growth processes; the thermophysical properties of complex fluids, such as ionic liquids and liquid crystals; the phase behavior of polymeric, colloidal, and self-assembled systems; and the synthesis, design and characterization of advanced materials, etc.

Taking this course, a motivated student will learn:

1. What quantities can be calculated using molecular simulations
2. Classical statistical mechanics, which is the theoretical basics of molecular simulations
3. Simple algorithms for two main molecular simulation methods, Molecular Dynamics and Monte Carlo
4. How to implement one of these algorithms for a basic system
5. How to use these methods implemented in popular open source tools



Who should enroll: the course is aimed for Ph.D. students, however **Master students** are also encouraged to enroll. Although the course is theoretical, it is expected that students focused on experimental work will also benefit. Experimentalists often have to deal with the literature data, obtained using molecular simulations, and this course will help them in making sense of the simulation results. The course is about the **methods** and not about any specific systems, so it could be of interest for students outside of ChemE, e.g. physics, chemistry, mechanical engineering, etc.