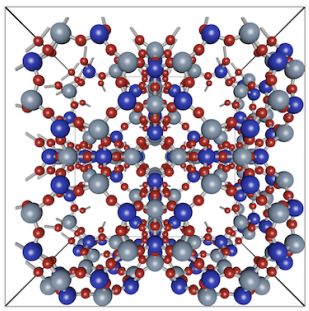
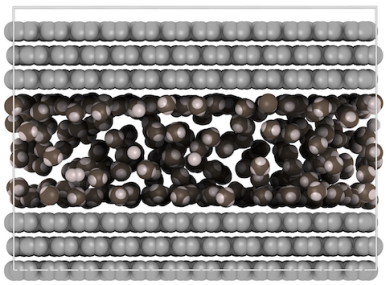
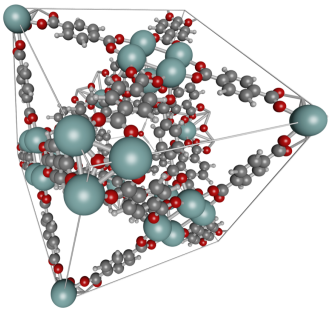
DEPARTMENT OF CHEMICAL AND MATERIALS ENGINEERING
UNDERGRADUATE / GRADUATE ELECTIVE COURSE

ChE 490/775: "Molecular Simulations in Chemical Engineering"

WHEN: SPRING 2022, WEDNESDAYS 6:00-8:50 PM
WHERE: CENTRAL KING BUILDING 215

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. How molecular dynamics and Monte Carlo methods work
3. How to implement one of these methods for a basic system
4. How to use these methods implemented in popular open source tools
5. How to use Python for data processing
6. How to use High Performance Computing facilities (available at NJIT) to run molecular simulations
7. How to search and study literature on molecular simulations
8. How to write reports on computational projects

Additional outcome:

The final project will be implemented in groups, and completed projects can result in journal publications. The course project from ChE 775 in 2020 was published in *J. Phys. Chem. B* https://doi.org/10.1021/acs.jpcb.0c10505

Who should enroll:

The course was initially designed for Ph.D. students, however **undergraduate** 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.

Instructor: Prof. Gennady Gor
Web: http://porousmaterials.net/ e-mail: gor@njit.edu