Fall 2020

CHEM 391-138: Research and Independent Study

Farnaz Shakib

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CEHM 391-138, Research and Independent Study - Fall 2020

Instructor: Farnaz A. Shakib, Ph.D.

Office: Tiernan 368
Email: shakib@njit.edu
Office Hours: M, W 11:00 am – 12:00 pm. And by appointment.

Textbook: There is no textbook for this course. Lecture notes will be provided for the students.

Course Content: Tentative material to be covered.

Discussion 1. Introduction to Nanoporous Materials
Discussion 2. 3D and 2D Metal-Organic Frameworks (MOF) as Separation Membranes
Discussion 3. Laying out the Project and Necessary Theoretical Knowledge/Computational Tools
Discussion 4. Introduction to Classical Molecular Dynamics
Discussion 5. Force Fields
Discussion 6. Constant Temperature/Pressure Simulations
Discussion 7. Introduction to LAMMPS as a Package for Simulation of Materials
Discussion 8. Building a MOF-based Separation Cell for LAMMPS
Discussion 9. Introduction to Bash Environment for Running Jobs
Discussion 10. Performing Simulations
Discussion 11. Introduction to Gnuplot and Analyzing Results
Discussion 12. Introduction to VESTA and Visualization of Results

Learning outcomes

After successful completion of the course students will
- understand the theoretical principles of MD simulations
- understand the significance of basic algorithms and their parameters for a successful simulation
- understand the basics of Bash/Linux environment for running calculations
- can run MD simulations using LAMMPS package
- can critically analyze the results of simulations
- can visualize the results of simulations using graphical interfaces

Final Evaluation

Students will make a presentation on the project they had performed during semester. They will be evaluated based on their understanding of MD simulations of materials, quality of their simulations, visualized data and oral presentation.
Grading:

Finishing-up a satisfactory level of simulation: 20%
Presentation (Introduction of MD simulations of materials): 20%
Presentation (Quality and diversity of the extracted results from simulations): 20%
Oral presentation: 40%

A (90-100%), B+ (85-89.9%), B (80-84.9%), C+ (75-79.9%), C (70-74.9%), D (60-69.9%), F(<60%)