

Fall 2020

CHEM 391-138: Research and Independent Study

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

Instructor: Farnaz A. Shakib, Ph.D.

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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%)