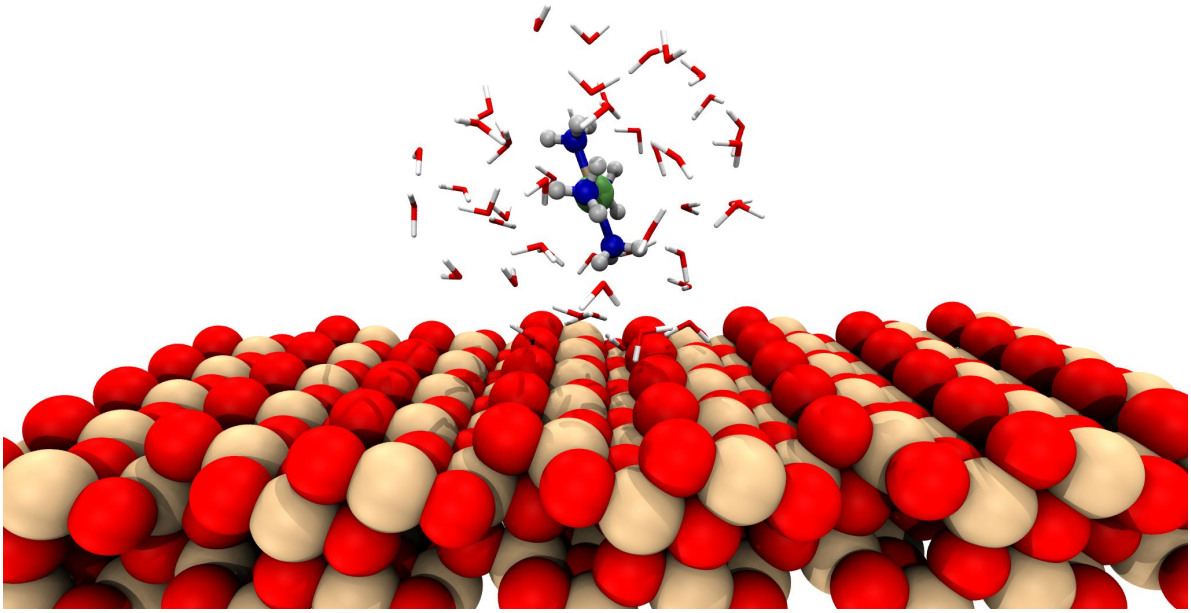
Institute for Computational Molecular Science Education

Fundamentals of Molecular Dynamics

July 8 – 12, 2024



Micron School of Materials Science and Engineering
Boise State University

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BOISE STATE UNIVERSITY

Organizing Committee

- **Eric Jankowski**, *Associate Professor,* Boise State University
- **Neeraj Rai**, *Associate Professor,* Mississippi State University
- **Jindal Shah**, *Associate Professor,* Oklahoma State University
- **Michael Shirts**, *Professor,* University of Colorado, Boulder
- **Sapna Sarupria**, *Associate Professor,* University of Minnesota
- **Amir Haji-Akbari**, *Assistant Professor,* Yale University
- **Rachael Skye**, *Graduate Student,* Cornell University
- **Hemanth Haridas**, *Postdoc,* University of Utah

Local Organizing Committee (Teaching Assistant / TA)

- **Tamar Burrell**, *Project Coordinator*, Mississippi State University
- **Maya Duratovic**, *Event Coordinator,* Boise State University
- **Arlind Kacirani (TA)**, *Graduate Student*, Yale University
- **Omar Khalifa (TA)**, *Graduate student*, Yale University
- **Barbara Morales (TA)**, *Graduate student*, University of Colorado Boulder
- **Chris Jones (TA),** *Graduate Student,* Boise State University
- **Marjan Albooyeh (TA)**, *Graduate Student*, Boise State University

Lecture Schedule: Monday, June 8

Location: MCMR

8:00 - 9:00 am: Breakfast

9:00 - 9:30 am: Welcome and pre-survey (Eric, Rich)

9:30 - 10:45 am: HPC Setup (Eric)

10:45 - 11:15 am: Break

11:15 - 12:30 pm: Theory 1 (Michael)

12:30 - 2:00 pm: Lunch

2:00 - 3:15 pm: Theory 2 (Michael)

3:15 - 3:45 pm: Coffee break

3:45 - 5:00 pm: Simple Fluids 1 (Rachael)

Lecture Schedule: Tuesday, June 9

Location: MCMR

8:00 - 9:00 am: Breakfast

9:00 - 10:15 am: Theory 3 (Michael)

10:15 - 10:30 am: Break

10:30 - 12:30 pm: Simple Fluids 2 (Rachael)

12:30 - 2:00 pm: Lunch

2:00 - 3:15 pm: Water 1 (Amir)

3:15 - 3:45 pm: Coffee break

3:45 - 5:30 pm: Analysis/Visualization (Eric)

Lecture Schedule: Wednesday, June 10

Location: MCMR

8:00 - 9:00 am: Breakfast

9:00 - 10:45 am: Water 2 (Amir)

10:45 - 11:15 am: Break

11:15 - 12:30 pm: Force Fields (Hemanth/Michael)

12:00 - 7:00 pm: Lunch and Choose-your-own-adventure

7:00 pm Dinner at the Ram/Stonehouse

Lecture Schedule: Thursday, June 1

Location: MCMR

8:00 - 9:00 am: Breakfast

9:00 - 10:45 am: DEI EmPower (Eric)

10:45 - 11:15 am: Break

11:15 - 12:30 pm: Polymers (Eric)

12:00 - 2:00 pm: Lunch

2:00 - 3:15 pm: Analysis/Visualization 2 (Eric)

3:15 - 3:45 pm: Coffee break

4:00 - 6:00 pm: Poster Session

Lecture Schedule: Friday, June 12

Location: MCMR

8:00 - 9:00 am: Breakfast

9:00 - 10:45 am: Advanced Topic Pointers (All)

10:45 - 11:15 am: Break

11:15 - 12:30 pm: Ask Us Anything (All)

12:30 - 12:45 pm: Post-Survey, Adjourn

Poster Session

Location: 106 MCMR

Breese, Jacob (The Ohio State University): Automating Simulations of Block Copolymers to Find Structural Features Using a Closed-Loop Optimization Process

Carolina Brindis Flores, Cristel (Rice University): Carbon-neutral recovery of natural gas from shale: Sequestering CO2 while enhancing gas production

Rickman, Maggie (Washington State University): Comparatively Testing CO Oxidation on Rh-Doped and Pt-Doped Copper-Based Catalysts

Nguyen, Thao (The University of Oklahoma): Effects of Surface-Active Agents on the Oil-Water Interface Dynamics under Non-Equilibrium Conditions

Boriwaye, Temitope (University Of Vermont): Electromigration Mitigation with Graphene Nano-ribbons and Metal Interfaces

Ranganath Prabhakar, Praveen (University of California Irvine): Estimation Of Free Energies Of Fkbp12-Ligand Systems Using Enhanced Sampling Methods

Naghshnejad, Pegah (Louisiana State University): Graph-Based Modeling and Molecular Dynamics for Ion Activity Coefficient Prediction in Polymeric Ion-Exchange Membranes

Shams, Elika (University of Connecticut): Investigating the structural difference of a mutation in tropoelastin with MD simulation

Szostak, Bogumiła (University of Silesia in Katowice): Mechanical micromanipulation of polymer chains

Ferguson, Matthew (Boise State University): Modeling the Living Genome

Abbasi, Nazanin (University of Arkansas): Molecular Dynamics Simulation of NaCl Nucleation on the Membrane Surface

Adepoju, Stephen (Northeastern University): Molecular Dynamics Simulations of Lipid Bilayer Mixtures: Developing Liposomes with Optimal Mechanical Properties

Ochieng, Sharon (Auburn University): Influence of Three-Body Effects on Halogen Bonding

Khang Bui, Quang (The University of Oklahoma): Solubility and diffusivity of aqueous hydrogen under kaolinite confinement