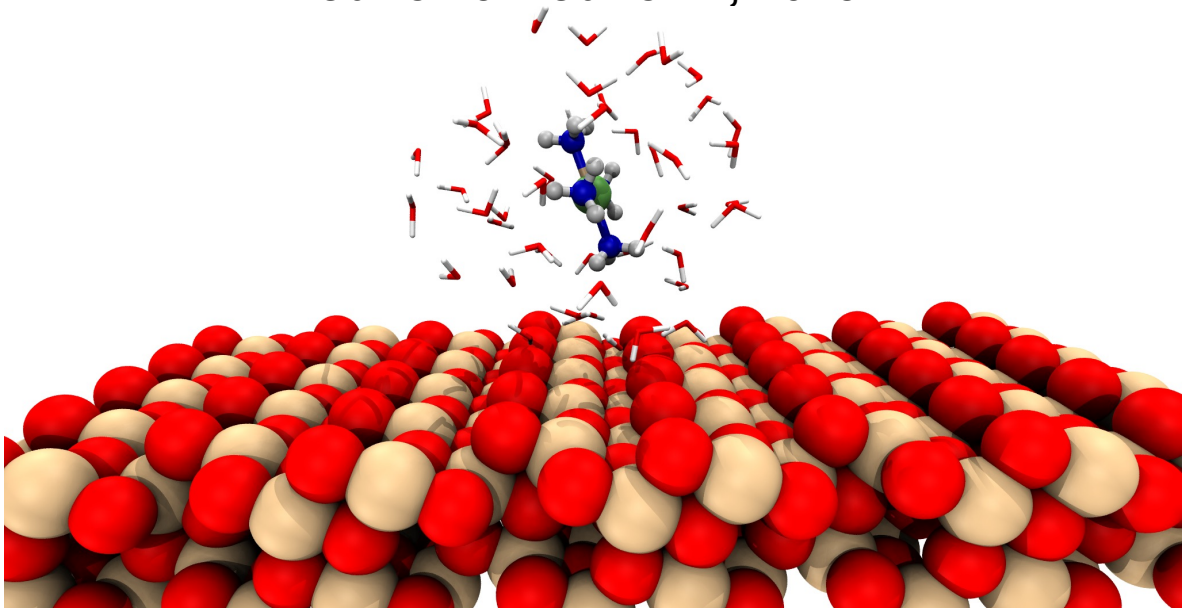
Institute for Computational Molecular Science Education

QM/MM and ab initio Molecular Dynamics Summer School

June 23 – June 27, 2025



School of Chemical Engineering
College of Engineering, Architecture and Technology
Oklahoma State University

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Organizing Committee

- **Eric Jankowski**, *Professor,* Boise State University
- **Neeraj Rai**, *Professor,* Mississippi State University
- **Sapna Sarupria**, *Associate Professor,* University of Minnesota
- **Jindal Shah**, *Professor,* Oklahoma State University
- **Michael Shirts**, *Professor,* University of Colorado, Boulder

Instructors

- **Mario Borunda**, *Professor ,* Oklahoma State University
- **Kwangho Nam**, *Associate Professor,* The University of Texas at Arlington
- **Phanish Suryanarayana**, *Professor,* Georgia Institute of Technology

Local Organizing Committee

- **Foyez Ahmed**, *Graduate Student*, Oklahoma State University
- **Masrur Ahmed**, *Graduate Student*, Oklahoma State University
- **Sudip Kumar Das**, *Graduate Student*, Oklahoma State University
- **Naserian Kambaine**, *Graduate Student*, Oklahoma State University
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- **Nuha Shouk,** *Graduate Student*, Oklahoma State University
- **Amey Thorat,** *Graduate Student*, Oklahoma State University
- **Ashutosh Verma,** *Graduate Student*, Oklahoma State University

Teaching Assistants

- **Sayan Bhowmik,** *Graduate Student*, Georgia Institute of Technology
- **Sudip Kumar Das,** *Graduate Student*, Oklahoma State University
- **Donghyuk Suh,** *Postdoctoral Researcher, Lehigh University*
- **Raafik Thodika,** *Graduate Student*, Oklahoma State University
- **Ashutosh Verma**, *Graduate Student*, Oklahoma State University

Administrative Support

- **Ms. Tamar Burrell,** Mississippi State University
- **Ms. Natalie Henderson,** Oklahoma State University
- **Mr. Patrick Wheeler,** Oklahoma State University

Lecture Schedule: Monday, June 23, 2025

Location: Engineering North 450

8:30 – 9:00 am: Check-in/refreshments

9:00 – 10:30 am : General Remarks - goals for the week (JS)
: Dr. Richard Mohn, Evaluation
: PSC Resources set-up, wifi set-up (EJ/JS)

10:30 – 10:50 am: Coffee Break

10:50 – 12:20 pm: Introduction to Molecular Dynamics (MD) (SS/EJ/JS)
: Simulation of LJ particles (SS/EJ/SS)

12:20 – 1:50 pm: Lunch

1:50 – 3:20 pm: Set-up of MD simulations of water & Analysis (SS/EJ/JS)

3:20 – 3:40 pm: Coffee Break

3:40 – 5:15 pm: Introduction to DFT (PS)
: Gas-phase calculations (PS)

Lecture Schedule: Tuesday, June 24, 2025

Location: Engineering North 450

8:30 – 9:00 am: Refreshments

9:00 – 10:30 am: Introduction to DFT Continued (PS/MB)
: Pseudopotential, Exchange-correlation functions

10:30 – 10:50 am: Coffee Break

10:50 – 12:20 pm: Set-up of an AIMD calculation for Ar (PS)
: Set-up of an AIMD calculation for water (PS)

12:20 – 1:50 pm: Lunch

1:50 – 3:20 pm: Analysis of AIMD trajectories and vibrational spectra (MB)

3:20 – 3:40 pm: Coffee Break

3:40 – 5:10 pm: Wrap-up, speed-up calculations (PS)

Lecture Schedule: Wednesday, June 25, 2025

Location: Engineering North 450

8:30 – 9:00 am: Refreshments

9:00 – 10:30 am: Interfacial calculations (PS)

10:30 – 10:50 am: Coffee Break

10:50 – 12:20 pm: ML potentials, Delta-XC approach (PS)

12:20 – 1:50 pm: Lunch

1:50 – 3:20 pm: Generation of Defects (MB)

3:20 – 3:40 pm: Coffee Break

3:40 – 5:10 pm: CHARMM/AMBER Build (DS)
: QM/MM Fundamentals (KN)

Location: Endeavor 2nd Floor

6:00 – 7:00 pm: Poster session

Lecture Schedule: Thursday, June 26, 2025

Location: Engineering North 450

8:30 – 9:00 am: Refreshments

9:00 – 10:30 am: Introduction to CHARMM GUI (DS)
: Build a system of protein in water (KN)

10:30 – 10:50 am: Coffee Break

10:50 – 12:20 pm: Molecular Mechanics minimization/equilibration (DS, KN)

12:20 – 1:50 pm: Lunch

1:50 – 3:20 pm: Enhanced sampling & umbrella sampling (KN)

3:20 – 3:40 pm: Coffee Break

3:40 – 5:10 pm: Analysis (DS, KN)

Location: Boomer Lake

6:00 – 9:00 pm: Picnic

Lecture Schedule: Friday, June 27, 2025

Location: Engineering North 450

8:30 – 9:00 am: Refreshments

9:00 – 10:30 am: QM/MM & ab initio QM/MM

10:30 – 10:50 am: Coffee Break

10:50 – noon: Ask Us Anything (MB, KN, NR, SS, JS)

noon – 12:15 pm: Post-workshop survey

12:15 pm: Adjourn

Poster Session

Location: Endeavor Second Floor

Almohri, Sayed (University of Michigan): Towards In Silico Zeolite Membrane Design Enabled by the ChIMES Interatomic Potential

Dumas, Adam (North Carolina State University): Polyoxymethylene Pyrolysis Models from Experiments and Reactive Molecular Dynamics

Foroozmehr, Maryan (University of California, Davis): Structural and Dynamic Insights into Antigenic Components of Chlamydia trachomatis for Universal Vaccine Design

Ghimire, Amar (University of North Texas): Exploring the Atomic Structure of Amorphous Oxides Using Classical and Ab Initio Simulations

Ibeto, Ifeanyi (The University of Alabama, Tuscaloosa): Predictive Modeling of Gas Diffusion Coefficients in Polymer Systems

Marabatha, Rishab (Oklahoma State University): Probabilistic Structural Clustering to Quantify Allosteric Response in Pyruvate Kinase

McKee, Job (Oklahoma State University): Balancing polar and non-polar interactions using condensed phase alcohol model refinement

Mooers, Blaine (University of Oklahoma Health Sciences Center): Quantum crystallography applied to RNA

Quach, Nhu (University of Minnesota): Molecular Insights into Electrolyte and Solvent Effects in Electro-Organic Reactions

Shouk, Nuha (Oklahoma State University): Threshold Displacement Energy (Ed) in CIGS

Yuan, Hao (University of Oklahoma): Hydrogen in Nanoporous Materials: A Computational Understanding of the Hard and Soft Matters