

7th Molecular Simulations Workshop

Northeastern Regional Edition

September 29, 2026

Invited Talks

1. **Dr. Noam Bernstein** — *Iterative Fine Tuning of MACE Foundation Models*
2. **Prof. Ian Bourg** — *Multiscale Simulation of Hydrated Clay Colloidal Assemblages*
3. **Prof. Gregory Dignon** — *Phase Separation, Mixing and Demixing in Biomolecular Systems*

Panel Discussion “How Should We Train the Next Generation of Computational Researchers?”

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| 1. Prof. Jerelle Joseph (Princeton, CBE) | 4. Prof. Alexander Urban (Columbia, CBE) |
| 2. Prof. Ashley Guo (Rutgers, CBE) | 5. Prof. Nutth Tuchinda (NJIT, CME) |
| 3. Prof. Michele Pavanello (Rutgers, Physics) | |

Poster Presentations

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| 1. Aditya Dilip Lele — <i>Development and Assessment of Curriculum Resources for Teaching Molecular Simulations and Their Applications</i> | 13. Santiago Flores Roman — <i>MezCal: An Efficient Monte Carlo Simulation Software for Dense and Nanoconfined Fluids</i> |
| 2. Diana Castaneda Bagatella — <i>Sign-Consistent Curvature-Driven Surface Hopping for Robust Non-Adiabatic Dynamics</i> | 14. Shahid Akbar — <i>From 2D to 3D designing of Electrically Conductive and Magnetically Bi-stable Coordination Polymers</i> |
| 3. Egor Demidov — <i>Is surface stress or surface free energy responsible for adsorption-induced deformation?</i> | 15. Shannon Zhang — <i>Asymmetric Effects Underlying Dynamic Heterogeneity in Miscible Blends of Poly(methyl methacrylate) with Poly(ethylene oxide)</i> |
| 4. Geordy Jomon — <i>Molecular Simulations of Organophosphorus Compounds: From Pure Species to Mixtures</i> | 16. Shogo Nakaza — <i>Exploring 2D metal-organic frameworks as next generation Li and Na-ion cathode materials</i> |
| 5. Kaelyn Chang — <i>Guiding Configurational Entropy Utilizing an Information-Theoretic Collective Variable</i> | 17. Sowmya Atukuri — <i>Mechanistic Investigation of Nanobubble-Assisted Water Washing for Enhanced Oil Removal from Contaminated Soil</i> |
| 6. Mansi Gokani — <i>Design considerations for polystyrene binding polypeptides</i> | 18. Trinh Quoc Dat Luong — <i>Mechanical Properties of Necks Between Primary Spheres in Carbonaceous Aggregates: A Molecular Dynamics Study</i> |
| 7. Margarita Gordiychuk — <i>Searching for Sequence Features that Control DNA Cyclizability</i> | 19. Tyler Oberholtzer — <i>Comparative Molecular Dynamics Simulation of Oxygen Nanobubble Behavior Using GRO-MACS and LAMMPS</i> |
| 8. Md Sojib Kaiser — <i>Entropic Pressure in Confined Active Vesicles</i> | 20. Udochukwu Laura Nwanebu — <i>Density Functional Theory Study of pH-Dependent Short-Chain PFAS Adsorption on Kaolinite and Montmorillonite Basal and Reactive-Edge Surfaces</i> |
| 9. Noor Aldin Alzghoul — <i>Reactive Molecular Dynamics Investigation of Polyethylene Pyrolysis Under Rapid Thermal Conditions</i> | 21. Vid Liam Stijelja — <i>A Comparative Study on Effects of Defects on Thermal Conductivity in Silicon</i> |
| 10. Ravindu L. Senevirathna — <i>Molecular Dynamics of Nanobubble Nucleation in Water: Effect of PFAS on Nanoscale Cavity Formation</i> | 22. Vladimir Grigorev — <i>Mesoscale Heterogeneity Shapes Molecular Selectivity and Transport in Biomolecular Condensates</i> |
| 11. Rubayet Hassan — <i>A Computational Model of Fluctuating Active Membranes: Implication for Entropic Pressure</i> | |
| 12. Sandip Bhusal — <i>Ring Polymer Liouville Equation: A Robust and Efficient Approach to Non-Adiabatic Dynamics</i> | |



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Program

- **9:00 – 9:15** Opening Remarks
- **9:15 – 10:00 Noam Bernstein** “Iterative fine tuning of MACE Foundation Models”
- **10:00 – 10:30** Coffee Break and Networking
- **10:30 – 11:15 Gregory Dignon** “Phase separation, mixing and demixing in biomolecular systems”
- **11:15 – 11:30** Group Photo
- **11:30 – 12:30 Panel Discussion** “How Should We Train the Next Generation of Computational Researchers?”
- **12:30 – 1:15** Lunch Break and Networking
- **1:15 – 1:45** Poster Pitch Presentations
- **1:45 – 3:15 Poster Session**
- **3:15 – 4:00 Ian Bourg** “Multiscale Simulation of Hydrated Clay Colloidal Assemblages”
- **4:00 – 4:15** Closing Remarks