



**Division of Physical Chemistry
American Chemical Society**

Rare Event Sampling in Material Science Problems: From Fundamental Understanding to Technological Applications

Omar Valsson
Gül H. Zerze
Organizers

Walter E. Washington Convention Center
See schedule for room locations

18-20 August 2025

PHYS Programs also available online:



MONDAY MORNING

Biomolecular Folding, Binding, & Conformational Transitions

Hall E, Room 20 | O. Valsson, *Presiding*

8:00 AM. Opening Remarks.

8:05 AM. Learning mechanisms of rare events from short-trajectory data. **A. Dinner**

8:35 AM. Rare event sampling as applied to artificial enzyme design. **S.D. Schwartz**

9:05 AM. From nanopores to proteins: Deciphering rare event kinetics and mechanisms using path sampling approaches. **A. Haji-Akbari**

9:35 AM. Enhanced sampling of ligand binding coupled to the RNA conformational dynamics. **R. Elangovan, D. Ray**

9:55 AM. Break.

10:15 AM. Data-driven enhanced sampling of minimum free energy pathways. R. Elangovan, S. Chatterjee, **D. Ray**

10:45 AM. Long-timescale simulation of protein interactions at atomic resolution in cell-like environment. **A. Singh**, A.M. Tytarenko, V.K. Ambati, M.M. Copeland, P. Kundrotas, P.O. Kasyanov, E.A. Feinberg, I. Vakser

11:15 AM. Exploring the free-energy landscape and transition paths for RNA folding/unfolding using a deep learning-driven simulation technique. **A. Gupta**, H. Ma, A. Ramanathan, G.H. Zerze

11:35 AM. Unraveling the dissociation kinetics of barnase-barstar complex in full atomistic detail. **D. Shrestha**, O. Valsson

11:55 AM. Closing Remarks.

MONDAY AFTERNOON

Biomolecular Complexes, Disordered Proteins, & Cryptic States

Hall E, Room 20 | G. H. Zerze, *Presiding*

2:00 PM. Opening Remarks.

2:05 PM. MELD x MD accelerator for protein molecular dynamics.

K.A. Dill, A. Bogetti, E. Brini, C. Liu, R. Nassar, S. Parui

2:35 PM. Fast sampling of protein conformational transitions.

M. Heyden

3:05 PM. How to stabilize (un)desirable conformations of disordered proteins. **G. Dignon**, Q. Jorgensen, V. Rodrigues

3:35 PM. Impact of different binding orientations of linker on PROTAC conformations: A computational comparative study of dBET6 and dBET23. **S. Bhusal**, A. Thompson, D. Walder, O. Valsson

3:55 PM. Break.

4:15 PM. Cracking undruggable proteins with cryptic pockets.

G. Bowman

4:45 PM. Enhanced sampling for cyclic peptides. **Y. Lin**

5:15 PM. Conformational instability of full-length staphylococcal protein a revealed by simulation and experiment. **K. Rahimi**, A. Halbing, R.C. Willson, G.H. Zerze

5:35 PM. Protocol for calculating binding affinity using artificial intelligence and umbrella sampling. **S. Kim**

5:55 PM. Closing Remarks.

TUESDAY MORNING

Materials & Catalysis

Hall E, Room 26 | D. Ray, *Presiding*

8:00 AM. Opening Remarks.

8:05 AM. Ethylene polymerization activity vs grafting affinity trade-off revealed by importance learning analysis of the CR/SiO₂ (Phillips) catalyst. C.A. Kim, A. Shayesteh Zadeh, **B. Peters**

8:35 AM. Enhanced sampling Monte Carlo techniques for simulation of concentrated antibody formulations and adsorption in porous materials. **H. Hatch**

9:05 AM. Studying long time scale behavior of transport in polymer membranes using statistically-inferred models of dynamics. N.S. Schwindt, B.J. Coscia, **M.R. Shirts**

9:35 AM. Enhanced sampling simulations for rare event characterization in sustainable materials design. **B. Yoon**

9:55 AM. Break.

10:15 AM. Materials applications of rare event sampling and free energy computation. **J. Whitmer**

10:45 AM. Machine learning models for accelerating transition state prediction in CO₂ reduction. **S. Yue**

11:15 AM. Intrinsic superconducting diode effect in tilted Weyl and Dirac semimetals. K. Chen, **B. Karki**, P. Hosur

11:35 AM. Closing Remarks.

WEDNESDAY MORNING

Machine Learning, Theory, & Mechanisms

Hall E, Room 26 | S. Yue, *Presiding*

8:00 AM. Opening Remarks.

8:05 AM. Exponentially tilted thermodynamic maps (expTM): Predicting phase transitions across temperature, pressure, and chemical potential. **P. Tiwary**

8:35 AM. Free energies from score-based generative models. **T. Bereau**

9:05 AM. Exploring constraint conformational ensemble with deep learning. **M. Chen**, Y. Liu, Y. Wang, Z. Yu, G. Lin, W. Jiang

9:35 AM. 2025 Young Investigator Awardee Advancing bottom-up mesoscopic modeling with coarse-graining and rare event sampling. **J. Jin**, D.R. Reichman

9:55 AM. Break.

10:15 AM. Progress in enhanced sampling and analysis of trajectories. **D.M. Zuckerman**

10:45 AM. Learning transition pathways using artificial neural networks. **C. Chipot**

11:15 AM. Characterizing phase transitions from sparse observations with thermodynamic maps. **L. Herron**, P. Tiwary

11:35 AM. Tunneling dynamics within Classical mechanics: An eikonal equation based approach. **B.K. Dey**

11:55 AM. Closing Remarks.

WEDNESDAY AFTERNOON

Nucleation, Crystallization, & Interfacial Liquids

Hall E, Room 25 | G. Dignon, *Presiding*

2:00 PM. Opening Remarks.

2:05 PM. Seeing the invisible in nucleation and achieving the inaccessible in capsid assembly. **S. Sarupria**

2:35 PM. Advances in the simulation of the nucleation of organic crystals. **E.E. Santiso**

3:05 PM. How do surfaces facilitate or inhibit the formation of ice?
A. Patel

3:35 PM. Break.

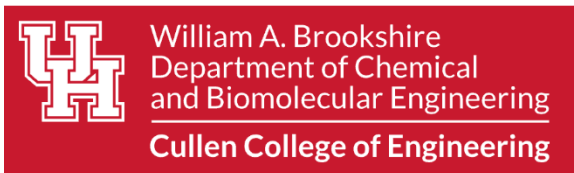
3:55 PM. Enhanced sampling and free-energy reconstruction for ion transport in water film: Logarithmic mean-force dynamics.
T. Morishita

4:25 PM. Optimizing on-the-fly probability enhanced sampling for complex RNA systems: Sampling free energy surfaces of an H-type pseudoknot. **K. Malekzadeh**, G.H. Zerze

4:45 PM. Investigating the dissociation mechanisms of 14-3-3/PMA2 protein complexes in the presence of stabilizing molecules via atomistic simulations. **O. Silva**, O. Valsson

5:05 PM. Closing Remarks.

The organizers acknowledge the following sponsor for their generous support:



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