Division of Physical Chemistry
American Chemical Society

Inferring Kinetics, Thermodynamics, and Mechanisms from Enhanced Sampling Simulations

Barak Hirshberg
GiovanniMaria Piccini
Organizers

San Diego Convention Center
see schedule for room locations

23-26 March 2025

PHYS Programs also available online:

SUNDAY MORNING

B. Hirshberg, *Presiding* | **Room 33C**

8:00 AM. Opening Remarks.

8:05 AM. Integrating path sampling with enhanced sampling for rare-event kinetics. **D. Ray**

8:35 AM. Sampling the transition path ensemble using a parallelizable path-integral-based algorithm. N. Malapally, L. Muellender, R. Andrea, M. Devodier, M. Parrinello, P. Carloni, **D. Mandelli**

9:05 AM. Finding optimal reaction coordinates from the projected dynamics of transition paths: A kinetic-based approach. **L. Mouaffac**, K. Palacio Rodriguez, F. Pietrucci

9:25 AM. Variational path sampling of rare dynamical events. **D. Limmer**

9:55 AM. Break.

10:15 AM. Enhanced sampling of dynamical trajectories. S. Falkner, A. Coretti, **C. Dellago**

10:45 AM. Short-time Infrequent Metadynamics for improved kinetics inference. **O. Blumer**, S. Reuveni, B. Hirshberg

11:05 AM. Good rates from bad coordinates. N. Mazzaferro, **P. Cossio**, G.M. Hocky

11:35 AM. Free-energy barriers and kinetic rates from short (non-ergodic) trajectories via Langevin models. **D.D. Girardier**, H. Vroylandt, S. Bonella, F. Pietrucci

11:55 AM. Closing Remarks.

SUNDAY AFTERNOON

G. Piccini, *Presiding* | **Room 33C**

2:00 PM. Opening Remarks.

2:05 PM. From enhanced sampling to nonequilibrium flux: Bridging scales with kinetic network analysis. **J.M. Swanson**

2:35 PM. Ad initio molecular dynamics and microkinetic modeling of a liquid catalysts: Propane dehydrogenation on liquid boron oxide. J. Tian, G.B. Collinge, S. Yuk, M. Lee, V. Glezakou, **R. Rousseau**

3:05 PM. Informed resetting: A strategy for accelerating molecular dynamics simulations. **J. Church**, O. Blumer, L. Ploutno, T. Keidar, S. Reuveni, B. Hirshberg

3:25 PM. Improving upon kinetics estimators for time-dependent and time-independent biases. N. Mazzaferro, P. Cossio, **G.M. Hocky**

3:55 PM. Break.

4:15 PM. From stability to dissociation: elucidating dissociation kinetics of protein-protein complexes via atomistic simulations. **O. Valsson**

4:45 PM. Data-driven path collective variables. **A. France-Lanord**

5:05 PM. Transition state identification of biomolecular dynamics via out-of-distribution detection in the hyperspherical latent space. **X. Huang**

5:35 PM. Accelerating transition dynamics simulation with recent advances in probabilistic machine learning. **Y. Du**

5:55 PM. Closing Remarks.

MONDAY MORNING
Thermodynamics

R. Capelli, *Presiding* | **Hall F, Room 4**

8:00 AM. Opening Remarks.

8:05 AM. Loop dynamics and catalysis in protein tyrosine phosphatases. **S.C. Kamerlin**

8:35 AM. Recent advances in machine learning collective variables. **L. Bonati**

9:05 AM. Identifying the order parameter for phase transitions in thermosalient materials for control. **H. Cuppen**, D. Galimberti, S. Ghasemlou, T. Rasing, X. Li

9:25 AM. Enhancing free energy methods by machine learning collective variables and equilibrium distributions. F. Dietrich, E. Olehnovics, **M. Salvalaglio**

9:55 AM. Break.

10:15 AM. Machine learning-based collective variables and GNN approaches for targeted dynamics and free energy manipulation in molecular and material systems. **D. Mendels**

10:45 AM. Harnessing enhanced sampling techniques to unravel molecular mechanisms of biomolecular processes in response to external stimuli. **F. Feixas**, H. Girame, C. Berga, A. John, H. Abes, M. Garcia Borras

11:05 AM. Exploring enzyme product release and enzyme-peptide conformational preferences with metadynamics. K. Croney, **J. McCarty**

11:35 AM. Enhanced sampling along the reaction coordinate by constrained molecular dynamics simulation. **J. Marks**, J. Gomes

11:55 AM. Closing Remarks.

TUESDAY MORNING
Thermodynamics

L. Bonati, *Presiding* | **Hall F, Room 4**

8:00 AM. Opening Remarks.

8:05 AM. Designing rare-event aware molecular simulations for drug discovery, force/energy learning and materials predictions. **S. Leoni**

8:35 AM. ab initio thermodynamics and beyond. B**. Cheng**

9:05 AM. Predicting biomolecular binding thermodynamics, kinetics and mechanisms through selective Gaussian accelerated molecular dynamics. **Y. Miao**

9:25 AM. Src and Abl kinase: A Milestoning study. **R. Elber**

9:55 AM. Break.

10:15 AM. Graph-driven strategy for enhanced sampling simulations of protein folding. Z. Fakhoury, S. Habershon, **G.C. Sosso**

10:45 AM. Explainable surrogate model-based collective variables for enhanced sampling. **S. Chatterjee**, D. Ray

11:05 AM. Multi-eGO: A structure-based approach to protein-ligand binding thermodynamics and kinetics. **R. Capelli**

11:35 AM. Art of automatic analysis for enhanced sampling simulations. N. Carton, V. Karunakaran Annapoorani, O.A. Petrisor, **N. Buchete**

11:55 AM. Closing Remarks.

TUESDAY AFTERNOON
Mechanisms

M. Podewitz, *Presiding* | **Hall F, Room 4**

2:00 PM. Opening Remarks.

2:05 PM. New route to the prebiotic synthesis of glycine via ab initio-based machine learning calculations. L. Huet, T. Devergne, **A. Saitta**

2:35 PM. Estimating mechanisms, free energies, and rates all at the same time. **R. Covino**

3:05 PM. Standard binding free energy estimates between photosystem I and ferredoxin isoforms in chlamydomonas reinhardtii using enhanced sampling molecular simulations. D. Sarkar, C. Fischer, D. Boren, S. Schmollinger, D. Strenkert, **J.V. Vermaas**

3:25 PM. Computing biopolymer–ligand binding free energy using lossless compression. **L. Simine**

3:55 PM. Break.

4:15 PM. Unveiling extreme chemistry in icy Giants' interiors through atomistic simulations. **F. Siro Brigiano**

4:45 PM. Understanding the conformational free energy landscape of drug-like molecules via enhanced sampling and unsupervised clustering. **A. Ferreira**, M. Salvalaglio

5:05 PM. Exploration of molecular structures and reaction pathways using adaptive learning and neural networks. **V. Glezakou**, M.Z. Makos, D. Zhang, R. Rousseau

5:35 PM. Investigating the microscopic adsorption process and mechanisms of solvated Li^+, Na^+, and K^+ in MOFs with an integrated theoretical and experimental approach, using MOF-808 as a case study. **Y. Pan**

5:55 PM. Closing Remarks.

WEDNESDAY MORNING
Mechanisms

D. Ray, *Presiding* | **Room 32A**

8:00 AM. Opening Remarks.

8:05 AM. Novel massively parallel path sampling approach applied to ab initio modeling of aqueous redox reactions and carbonic acid formation. D.T. Zhang, **T.S. van Erp**

8:35 AM. Withdrawn/break.

9:05 AM. Nuclear quantum effects and the Grotthuss mechanism dictate the pH of water. **S. Dasgupta**, F. Paesani

9:25 AM. Synergizing enhanced sampling and machine learning strategies in molecular simulation for representing and deploying high-dimensional free energy surfaces and learning reaction coordinates for conformational transformations of systems in explicit solvent. **M.E. Tuckerman**

9:55 AM. Break.

10:15 AM. Studying electrocatalytic selectivity of the oxygen reduction reaction (ORR) using ab initio free energy sampling. **E. Diesen**, A.M. Dudzinski, K. Reuter, V.J. Bukas

10:45 AM. Withdrawn/break.

11:05 AM. Towards predictive and operando computational catalysis: Examples from transition-metal chemistry. **M. Podewitz**

11:35 AM. Enhanced sampling simulations for transformative materials design and discovery in energy and sustainability challenges. **B. Yoon**

11:55 AM. Closing Remarks.

The organizers acknowledge the following sponsors for their generous support:

The Journal of Chemical Physics

TEL AVIV UNIVERSITY אוניברסיטת תל אביב