Division of Physical Chemistry
American Chemical Society

Computational & Theoretical Modeling of Biomolecular Dynamics in Crowded Environments

Taras Pogorelov
Matthias Heyden
Organizers

San Diego Convention Center
Room 33B (Mon – Wed)
Hall G/H, Room 9 (Thu)

24-27 March 2025

PHYS Programs also available online:

MONDAY AFTERNOON

Biomolecular Interactions in Crowded Environments

H. W. Hatch, M. Kozlowska, *Presiding*

2:00 PM. Opening Remarks.

2:05 PM. Ubiquity and importance of nonspecific intermolecular interactions in a crowded medium. **A. Minton**

2:40 PM. Ligand binding to cryptic sites with flexible side chains. **S. Vajda**, M. Lazou, D. Kozakov, D. Joseph-Mccarthy1

3:10 PM. Break.

3:20 PM. Exploring drug-target interactions in crowded environments by Brownian and molecular dynamics simulation. **R.C. Wade**

3:50 PM. PEG-mCherry interactions beyond classical macromolecular crowding. L. Haas-Neill, K. Joron, E. Lerner, **S. Rauscher**

4:20 PM. Coarse-grain modeling of monoclonal antibodies in high concentration formulations. **H.W. Hatch**, C. Bergonzo, M.A. Blanco, G. Yuan, S. Grudinin, M. Lund, J.E. Curtis, A. Grishaev, Y. Liu, V.K. Shen

4:50 PM. Break.

5:00 PM. Coarse-grained simulations of protein-protein interactions toward understanding the functionality of biomolecular assemblies. **M. Kozlowska**

5:30 PM. Decoding sequence-specific conformational transitions of disordered proteins in phase separation. **J. Mittal**

TUESDAY MORNING

All-Atom Simulations & Beyond

T. V. Pogorelov, J. A. Hadden-Perilla, *Presiding*

8:00 AM. Impact of physiological factors on the conformational dynamics and aggregation of amyloid-β. **B. Strodel**

8:30 AM. Fast calculation of small-angle scattering profiles of dense protein solutions modeled at the all-atom level. S. Qin, **H. Zhou**

9:00 AM. Investigating aggregation mechanisms of alpha-synuclein using molecular dynamics through local water dynamics. **M.A. Rothermund**, V. Vaissier Welborn

9:20 AM. Break.

9:30 AM. In-cell protein-protein interactions and protein folding dynamics. P.P. Samuel, M. Gruebele, **T.V. Pogorelov**

10:00 AM. How crowding affects the dynamics and activity of the hepatitis C virus NS3/4A protease. N. Ostrowska, M. Lobka, A. Popielec, M. Wojciechowska, M. Feig, **J. Trylska**

10:30 AM. Understanding biochemical processes in complex environments through dynamical networks. **C. Calvó-Tusell**, F.L. Kearns, N.A. Wauer, A.C. Dommer, L. Casalino, R.E. Amaro

10:50 AM. Break.

11:00 AM. Mechanistic insights into HBV capsid assembly and its inhibition revealed by all-atom MD simulations. C. Pérez-Segura, M. Hagan, A. Zlotnick, **J.A. Hadden-Perilla**

11:30 AM. Impact of crowding on protein conformational free energy landscapes. **M. Heyden**

TUESDAY AFTERNOON

Molecular Models of Cells & Intracellular Dynamics in Crowded Environments

E. Deeds, B. Zhang, *Presiding*

2:00 PM. Molecular dynamics simulation of an entire cell. **S. Marrink**, C. Brown, J. Stevens

2:30 PM. How do macromolecular crowding environments affect enzyme activities?. **Y. Sugita**

3:00 PM. DNA condensation and aggregation induced by polyamine and protamine. **Y. Lansac**, Y. Jang

3:20 PM. Break.

3:30 PM. Macromolecular assembly in crowded environments. L. Lagunes, K. Ghabra, G. Ordonez, S. Grudinin, **E. Deeds**

4:00 PM. Multiscale simulations of biomolecular processes in disease. **A. Yu**

4:30 PM. Structural and thermodynamic features of HIV-1 capsid self-assembly. **L. Foglia**, D.E. Santos, A. Yu

4:50 PM. Break.

5:00 PM. Near-atomistic modeling of the spatial environment of a single gene. **B. Zhang**

5:30 PM. Deconstructing structural mechanisms of metabolon formation. **P.P. Samuel**, T.V. Pogorelov, M. Gruebele

WEDNESDAY MORNING

Multiscale Modeling of Biomolecular Systems

J. Kelz, F. Sterpone, *Presiding*

8:00 AM. Multi-resolution simulations of biological systems. **A. Aksimentiev**

8:30 AM. No ring to rule them all: facing and leveraging the multiscale nature of proteins to model them at the right level of detail. **R. Potestio**

9:00 AM. Architecting megamolecule self-assembly networks: Insights from coarse-grained simulations and design strategies. **J. Wu**, **Z. Gu**, J.A. Modica, **S. Chen**, M. Mrksich, G.A. Voth

9:20 AM. Break.

9:30 AM. Proteome dynamics at the cell-death temperature: a picture of life adaptation to different thermal niches. **F. Sterpone**

10:00 AM. Clarifying cataract: Modeling the dynamic molecular basis of aggregation in eye lens proteins. **J. Kelz**, J.A. Freites, D. Tobias

10:20 AM. Water structure and dynamics in polysaccharide (alginate) solutions and gels. A.A. Agles, **I.C. Bourg**

10:40 AM. Break.

10:50 AM. Performance efficient macromolecular mechanics via sub-nanometer shape based coarse graining. **J.R. Perilla**

11:20 AM. About the multiple mechanisms by which proteins associate with membranes. **M. Dal Peraro**

WEDNESDAY AFTERNOON

From Molecules to Cells: Machine Learning & Mathematical Models

M. Heyden, D. Kihara, *Presiding*

2:00 PM. Machine learning potentials toward next-generation biomolecular simulations. **G. De Fabritiis**

2:30 PM. Biomolecular representations for physics-based deep learning models. **A. Singharoy**

3:00 PM. Break.

3:10 PM. Building and Validating Structure Models from medium to low resolution cryo-EM Maps. **D. Kihara**

3:40 PM. Break.

4:10 PM. Investigating conformational mechanisms of STING activation: A computational approach. H. Gates, **M. Watanabe**

4:30 PM. Break.

4:40 PM. E. coli whole-cell modeling project. **M. Covert**

5:10 PM. Bringing a cell to life on a computer and in Minecraft. **Z. Luthey-Schulten**

THURSDAY MORNING

Intrinsic Disorder & Phase Separation

D. Potoyan, W. Zheng, *Presiding* | **Hall G/H, Room 9**

8:00 AM. Using both experimental and all-atom simulation data in training a coarse-grained model for disordered proteins. **R.B. Best**

8:30 AM. Protein association in a crowded environment: Resolution of models and interactions. **M. Biswas**

9:00 AM. Self-assembly of the tau protein: liquid-liquid phase separation and fibrillization. **J. Shea**

9:30 AM. Break.

9:40 AM. Uncovering residue-level driving forces underlying protein liquid-liquid phase separation. **S. Rekhi**, J. Mittal

10:00 AM. Collective behaviors emerging from dynamic complexity in self-organizing molecular systems. **G. Pavan**

10:30 AM. Break.

10:40 AM. Exploring structural features of intrinsically disordered proteins. **W. Zheng**

11:10 AM. Molecular drivers of aging in biomolecular condensates. **D. Potoyan**

11:40 AM. Closing Remarks.