

Biophysical Society 69th Annual Meeting
Theory & Computation Subgroup Symposium
Saturday February 15, 2025
Los Angeles, California

Subgroup Chair: Benoit Roux, University of Chicago, USA

Symposium Time: 8:30 AM-12:30 PM PST

Symposium Room: Petree Hall D

Subgroup Business Meeting: 12:00 PM

8:30 PM Opening Remarks

8:35 AM Grant Rotskoff, Stanford University, USA

Building Efficient and Transferable Generative Models of Intrinsically Disordered Protein Conformational Ensembles

9:05 AM Andela Saric, Institute of Science and Technology Austria (ISTA), Austria

Modelling the Cell with Beads and Springs

9:35 AM **Mid-Career Award Talk:** Rommie Amaro, University of California, San Diego, USA

Multiscale Computational Microscopy

10:05 AM Break

10:20 AM Prabhu Raman, Nurix Therapeutics, USA

Physics-Based Modeling of Ternary Complexes Driving Targeted Protein Degradation

10:50 AM Flash Talks:

Seonghan Kim, Oak Ridge National Laboratory, Tennessee, USA.

Modeling and simulation of bio-polymer interface

Ehsan Khodadadi, University of Arkansas, USA.

Optimizing liposomal drug delivery systems through cholesterol dynamics: insights from coarse-grained simulations

Steven Ayoub, University of California, Irvine, USA.

Implicit solvent: Faster convergence, fewer technical issues for absolute binding free energy calculations (ABFE)

Amanda D. Stange, Aarhus University & Novo Nordisk Foundation, Aarhus, Denmark.

Exploring insulin-receptor dynamics: stability and binding mechanisms.

Haley Michel, Virginia Tech, Virginia, USA.

Advancing drug targeting of DNA and RNA structures using polarizable mixed-solvent simulations

11:05 AM **Early-Career Award Talk:** Denise Okafor, Penn State University, USA

Ligand-Driven Allostery in Nuclear Receptors

11:30 AM Aditi Borkar, University of Nottingham, UK

Cryo-OrbiSIMS Enables Integrative Modelling of RNA Structures at Atomic Resolution

11:55 AM Closing Remarks

12:00 PM Business Meeting

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