

Biophysical Society 67<sup>th</sup> Annual Meeting  
Theory & Computation Subgroup Symposium  
Saturday February 18, 2023  
San Diego, California

**Subgroup Chair:** Gregory A. Voth, University of Chicago, USA

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

**Symposium Room:** 6A

**Subgroup Business Meeting:** 12:00 Noon

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8:30 AM Opening Remarks

8:35 AM Margaret E. Johnson, Johns Hopkins University, USA

*Bending Membranes Along Distinct Pathways of Protein Assembly*

9:05 AM Juyong Lee, Seoul National University, South Korea

*Accurate Prediction of Protein-Ligand Interactions by Combining Physical Energy Functions and Graph-neural Networks*

9:35 AM Frauke Graeter, Heidelberg University, Germany

*Incorporating Chemistry into Classical Molecular Dynamics Simulations of Proteins by Machine Learning*

10:05 AM Break

10:20 AM Yuji Sugita, RIKEN, Japan

*Multi-Scale Molecular Dynamics Simulations of Macromolecular Crowding Effects and Regulation of Biomolecular Condensates*

10:50 AM **Mid-Career Award Talk:** Xuhui Huang, University of Wisconsin–Madison, USA

*Generalized Master Equation Models to Study Functional Dynamics of Proteins*

11:20 AM Janice Robertson, Washington University in St. Louis, USA

*Building a Molecular Model for Ion Channel and Transporter Stability in Membranes through a Partnership of Experiments and Computation*

11:50 AM Closing Remarks

12:00 Noon Subgroup Business Meeting

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