

Biophysical Society 66th Annual Meeting
Theory & Computation Subgroup Symposium
Saturday February 19, 2022
San Francisco, California

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

Symposium Time: 1:30 PM - 5:30 PM PST

Symposium Room: Moscone South 207/208

Subgroup Business Meeting: 5:00 PM

1:30 PM Pratyush Tiwary, University of Maryland

From Atoms to Emergent Mechanisms with AI-Augmented Molecular Simulations

2:00 PM Cecilia Clementi, Free University of Berlin, Germany

Learning molecular models from machine learning and experimental data

2:30 PM John Jumper, Google, United Kingdom

Highly Accurate Protein Structure Prediction with AlphaFold

3:30 PM Pilar Cassio, Flatiron Institute

Transition Rates, Survival Probabilities, and Quality of Bias from Time-dependent Biased Simulations

4:00 PM Daniel Zuckerman, Oregon Health & Science University

How Should We Think About Mechanism?

4:30 PM Edward Lyman, University of Delaware

Small differences with big effects: How lipid chemistry determines membrane curvature and viscosity

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