Contribution ID: **35** Type: **Oral contribution**

Bridging Scales in Molecular Simulations: Data-Driven Characterization of Free Energy Landscapes

Friday 11 July 2025 09:00 (50 minutes)

Understanding biomolecular behavior across multiple spatial and temporal scales remains a central challenge in molecular biophysics. Atomistic simulations offer fine-grained detail, but are computationally expensive, while coarse-grained models provide efficiency at the cost of resolution. Bridging these scales requires robust frameworks to translate between models and ensure consistent thermodynamic behavior across representations.

In this talk, I will present recent work on data-driven characterization of free energy landscapes, highlighting how machine learning and dimensionality reduction techniques can be used to identify relevant collective variables and thermodynamic basins from simulation data. I will then discuss how these insights can be transferred between atomistic and coarse-grained descriptions, enabling multiscale modeling of complex systems such as multy-body biomolecules.

Author: KUKHARENKO, Oleksandra (Max Planck Institute for Polymer Research)

Presenter: KUKHARENKO, Oleksandra (Max Planck Institute for Polymer Research)