Contribution ID: **20** Type: **Oral contribution**

Enhanced Artificial Intelligence Molecular Mechanism Discovery of Reaction Paths in Complex Systems

Friday 11 July 2025 09:50 (30 minutes)

Self-organization of molecules into ordered structures is crucial for both living and non- living matter. Artificial Intelligence Mechanistic Molecular Discovery[1] is an autonomous transition path sampling algorithm that uses deep learning to discover the underlying reaction mechanism of such molecular self-organizing phenomena. The algorithm uses the outcome of unbiased dynamical trajectories to construct, validate and update the quantitative mechanistic model. With the learned mechanistic model, the sampling of mechanistic trajectories or rare events can be enhanced, completing the cycle. Here, we enhance the method by including all potentially possible configurations in the reweighted path ensemble. We illustrate the novel methodology on simple potentials and a more complex molecular system.

[1] Jung et al., Nat. Comput. Sci. 3, 334–345 (2023).

Authors: Prof. BOLHUIS, Peter (University of Amsterdam); BREEBAART, Rik (University of Amsterdam)

Co-authors: Mr LAZZERI, Gianmarco (Frankfurt Institute for Advanced Studies); Prof. COVINO, Roberto (Goethe University Frankfurt)

Presenter: BREEBAART, Rik (University of Amsterdam)