Contribution ID: **8** Type: **Oral contribution**

Enhancing Molecular Simulations by Integrating Machine Learning and Quantum Computing

Wednesday 9 July 2025 09:50 (30 minutes)

The rare event problem often limits practical applications of classical Molecular Dynamics simulations. While powerful enhanced sampling techniques have been proposed and successfully applied to many important study cases, these methods typically require a suitable choice of collective variables (CVs) in input. This feature introduces systematic errors that are hard to estimate a priori. In this talk, we shall discuss a novel approach to enhanced sampling that does not require any CV in input. Instead, it relies on a combination of generative AI and uncharted exploration to enhance sampling in a fully data-driven way and to renormalization group techniques to use the generated data to represent equilibrium dynamics. In the resulting theory, path sampling can be further enhanced by resorting to quantum annealing machines, which enable the storage of the entire transition path ensemble in a single quantum computer's wave function.

Author: FACCIOLI, Pietro (University of Milan-Bicocca)

Presenter: FACCIOLI, Pietro (University of Milan-Bicocca)