Machine-learning acceleration for semiclassical and nonadiabatic dynamics

Jeremy Richardson

ETH Zurich

Semiclassical dynamics methods offer the promise of capturing quantum effects in large systems. However, when applied to complex molecules on the fly, they can be even more expensive than ab initio molecular dynamics. I will discuss how machine-learning techniques developed for accelerating ab initio molecular dynamics can be extended to provide the properties required for semiclassical approaches such as the ring-polymer instanton theory of tunnelling [1-3] and surface-hopping simulations of nonadiabatic processes [4].

References:
[1] G. Laude, D. Calderini, D.P. Tew & J.O. Richardson. "Ab initio instanton rate theory made efficient using Gaussian process regression." Faraday Discuss. 212, 237-258 (2018).
[2] W. Fang, Y.-C. Zhu, Y.-H. Cheng, Y.-P. Hao & J.O. Richardson. "Robust Gaussian Process Regression method for efficient tunneling pathway optimization: Application to surface processes." J. Chem. Theory Comput. 20, 3766-3778 (2024).
[3] S. Käser, J.O. Richardson & M. Meuwly. "Transfer Learning for Affordable and High-Quality Tunneling Splittings from Instanton Calculations." J. Chem. Theory Comput. 18, 6840-6850 (2022).
[4] J.O. Richardson. "Machine learning of double-valued nonadiabatic coupling vectors around conical intersections." J. Chem. Phys. 158, 011102 (2023).