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# Machine Learning Approaches for Thermodynamic and Kinetic Analysis of Molecular Systems

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**As a computer simulation tool, molecular dynamics (MD) can offer insight into chemical and physical processes, and plays a prominent role in computational chemistry, statistical physics, molecular biology, etc. With the rapid development of computers, the quantitative analysis of complex molecular systems based on large-scale MD simulations becomes a challenging problem. In this talk, I will introduce my recent works on machine learning based techniques for modeling and analyzing MD data, including variational approach for model reduction of molecular kinetics and normalizing flows for exploration of the energy landscape, which can overcome limitations of current data-driven approaches and help to advance the understanding of molecular thermodynamics and kinetics.**