

Inclusion of Machine Learning Kernel Ridge Regression Potential Energy Surfaces in On-the-Fly Nonadiabatic Molecular Dynamics Simulation

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We discuss a theoretical approach that employs machine learning potential energy surfaces (ML-PESs) in the nonadiabatic dynamics simulation of polyatomic systems by taking 6-aminopyrimidine as a typical example. The Zhu-Nakamura theory is employed in the surface hopping dynamics, which does not require the calculation of the nonadiabatic coupling vectors. The kernel ridge regression is used in the construction of the adiabatic PESs. In the nonadiabatic dynamics simulation, we use ML-PESs for most geometries and switch back to the electronic structure calculations for a few geometries either near the S_1/S_0 conical intersections or in the out-of-confidence regions. The dynamics results based on ML-PESs are consistent with those based on CASSCF PESs. The ML-PESs are further used to achieve the highly efficient massive dynamics simulations with a large number of trajectories. This work displays the powerful role of ML methods in the nonadiabatic dynamics simulation of polyatomic systems.

References

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