Towards Exact Molecular Dynamics Simulations with Quantum Chemistry and Machine Learning

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I will discuss an efficient symmetric gradient-domain machine learning (sGDML) approach for constructing next-generation CCSD(T)-quality interatomic force fields for molecules. The sGDML implementation is able to reproduce global potential-energy surfaces of intermediate-sized molecules with an accuracy of 0.1 kcal/mol using only few hundred molecular conformations for training. We demonstrate this accuracy for *ab initio* molecular dynamics (AIMD) trajectories of molecules, including toluene, naphthalene, ethanol, uracil, and aspirin. The GDML approach enables quantitative molecular dynamics simulations with quantum electrons and nuclei for molecules at a fraction of cost of explicit AIMD calculations, thereby allowing to achieve unprecedented insights into (thermo)dynamics of molecules [1,2].

References:

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[2] *S. Chmiela, H. E. Sauceda, K. R. Mueller, and A. Tkatchenko*, Towards exact molecular dynamics simulations with machine-learned force fields. **Nature Commun.** 9, 3887 (2018).