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Machine Learning of Accurate Energy-Conserving Molecular Force Fields STEFAN CHMIELA, Machine Learning Group, Technische Universität Berlin, ALEXANDRE TKATCHENKO, University of Luxembourg, HUZIEL SAUCEDA, Fritz-Haber-Institut der Max-Planck-Gesellschaft, IGOR POLTAVSKY, University of Luxembourg, KRISTOF SCHÜTT, KLAUS-ROBERT MÜLLER, Machine Learning Group, Technische Universität Berlin, GDML COLLABORATION — Efficient and accurate access to the Born-Oppenheimer potential energy surface (PES) is essential for long time scale molecular dynamics (MD) simulations. Using conservation of energy – a fundamental property of closed classical and quantum mechanical systems – we develop an efficient gradient-domain machine learning (GDML) approach to construct accurate molecular force fields using a restricted number of samples from ab initio MD trajectories (AIMD). The GDML implementation is able to reproduce global potential-energy surfaces of intermediate-size molecules with an accuracy of 0.3 kcal/mol for energies and 1 kcal/mol/Å for atomic forces using only 1000 conformational geometries for training. We demonstrate this accuracy for AIMD trajectories of molecules, including benzene, toluene, naphthalene, malonaldehyde, ethanol, uracil, and aspirin. The challenge of constructing conservative force fields is accomplished in our work by learning in a Hilbert space of vector-valued functions that obey the law of energy conservation. The GDML approach enables quantitative MD simulations for molecules at a fraction of cost of explicit AIMD calculations, thereby allowing the construction of efficient force fields with the accuracy and transferability of high-level ab initio methods.

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