From Atomistic, to Coarse-grained, to Generative Models based on Experimental Data

Julija Zavadlav[1]

[1]Technical University of Munich, Germany

Machine learning potentials (MLPs) are closing the gap between quantum-mechanical accuracy and the efficiency of classical force fields in materials modeling. In this talk, I will highlight key achievements of graph neural network-based atomistic and coarse-grained MLPs in capturing many-body physics and address current bottlenecks: achieving beyond density functional theory level accuracy and deploying MLPs at massive spatiotemporal scales. To address these challenges, I will introduce a range of innovative strategies that encompass synergistic integration of experimental and ab initio data, physics-based functional forms, and solvent-dependent molecular models. Through insightful case studies of various materials, I will demonstrate the practical effectiveness and versatility of our approaches. Additionally, our software platform chemtrain facilitates machine learning potential training with customizable routines and advanced training algorithms, while the extension chemtrain-deploy, enables scalable model-agnostic parallelization across multiple GPUs and million-atom simulations. Finally, I will show how coarse-grained (CG) MLPs combined with Boltzmann Generators (CG-BG) can achieve simulation-free equilibrium sampling of molecular systems with explicit solvent (atomistic) accuracy, thereby circumventing the scalability issue of classical BGs.