Modeling materials with machine learning potentials, and how to fine-tune them with active learning

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Machine learning (ML) integrated into computational chemistry research has paved the way for transformative advancements, rapidly propelling our ability to predict new molecules, materials, and processes with the desired properties.

At the core of our efforts lies the Amsterdam Modeling Suite (AMS), a versatile framework facilitating exploration across multiple levels of theory from DFT to force fields, providing invaluable insights into potential energy surfaces (PESs) and mechanical and electronic properties. The AMS driver orchestrates advanced PES explorations and molecular dynamics (MD) with as well as Grand Canonical Monte Carlo (GCMC), harnessing energies and forces obtained from engines.

With this set up you can use electronic structure methods as well as (machine learned) force fields to calculate a wide range of properties and processes such as reaction rates, conformer populations, sorption isotherms, viscosity, stress tensors, thermodynamic stability, and chemical vapor deposition.

Use the AMS driver with on-the-fly machine-learned potentials like NEquIP[1] as well as preparametrized ML potentials such as ANI-1ccx[2], M3GNet[3], [3] and CHGNet[4] to efficiently calculate relevant molecules, materials, and processes for various applications such as batteries, catalysis, polymers, and carbon capture and storage. AMS's ParAMS module exemplifies a comprehensive framework for constructing training data from DFT engines and optimizing ReaxFF and DFTB parameters. Through the integration of active learning in ParAMS workflows, researchers can quickly create and refine machine learning potentials to tackle their diverse chemistry and materials optimization challenges.

As an example, we will demonstrate how the universal neural network potential M3GNet can predict critical properties of battery materials like intercalation energies and diffusion barriers, enabling faster materials screening to accelerate the innovation in the energy storage domain. While out of the box M3GNet predictions are reasonable, fine-tuning the M3GNet potentials gives access to DFT-level accuracy also for activated processes such as Li diffusion.

We would like to discuss with you how to collaboratively shape future developments where we envisage a dynamic landscape where AMS, bolstered by ML advancements, stands as a catalyst for transformative materials research, propelling innovation across multiple domains.

[1] S. Batzner et al. Nature Comm. (2022), 13:2453
[2] J. S. Smith et al. Nature Comm. (2019), 10:2903
[3] C. Chen, S. Ong, Nature Comp. Sci. (2022), 2, 718-728
[4] B. Deng et al. arXiv:2302.14231 (2023)

<u>Keywords</u>: Materials modeling, machine learning, batteries.