Deep Modeling for Molecular Simulation

Hands-on 2-day virtual workshop

Dates: July 7-8, 2022

Program:

Day 1

- Morning - Introductory lectures
- Afternoon - Hands-on tutorial session 1 (Basic tools - Learning the potential energy surface using DeePMD-kit, LAMMPS, and Quantum ESPRESSO)

Day 2

- Morning - Introductory lectures
- Afternoon - Hands-on tutorial session 2 (Concurrent learning using DP-GEN, learning of Wannier centers with DeePMD-kit, and training models with long range interactions using DPLR)

Speakers:

- Weinan E (Peking University), Darrin York (Rutgers University), Robert DiStasio (Cornell University), Roberto Car (Princeton University)

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