A Pre-trained Deep Potential Model For Sulfide Solid Electrolytes With Broad Coverage and High Accuracy

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Solid electrolytes with fast ion transport are one of the key challenges for solid state lithium metal batteries. To improve ion conductivity, chemical doping has been the most effective strategy, and atomistic simulation with machine-learning potential helps find optimized doping by predicting ion conductivity for arbitrary composition. Yet most existing machine-learning models are trained on narrow chemistry, and new model has to be trained for each system, wasting transferable knowledge and incurring significant cost. Here, we propose a pre-trained deep potential model purpose-built for sulfide electrolytes with attention mechanism, known as DPA-SSE. The training set encompasses 15 elements and consists of both equilibrium and extensive out-of-equilibrium configurations. DPA-SSE achieves a high energy resolution of less than 2 meV/atom for dynamical trajectories up to 1150 K, and reproduces experimental ion conductivity of sulfide electrolytes with remarkable accuracy. DPA-SSE exhibits good transferability, covering a range of complex electrolytes with mixes of cation and anion atoms. Highly efficient dynamical simulation with DPA-SSE can be realized by model distillation which generates a faster model for given systems. DPA-SSE also serves as a platform for continuous learning, and the model fine-tune requires only a portion of downstream data. These results demonstrate the possibility of a new pathway for AI-driven development of solid electrolytes with exceptional performance.

References

1. R. Wang, M. Guo, Y. Gao, X. Wang, Y. Zhang, B. Deng, X. Chen, M. Shi, L. Zhang, Z. Zhong Arxiv:2406.18263 (2024)