Recent developments and applications of the machine-learned moment tensor potentials

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1. Introduction

Machine learning interatomic potentials (MLIPs) have emerged as a powerful approach for atomistic simulations which allows one to perform large-scale simulations with high (usually near density-functional theory) accuracy. Among different MLIPs, the moment tensor potential model (MTP) [1] has established itself among the most accurate, efficient, and widely used [2].

This work highlights a number of recent methodological developments in MTP construction and also a number of applications, where MTPs were used to model materials. In particular, while initial MTP model, implemented in the MLIP-2 package, was purely local [3], recently, it was shown how to incorporate long-range interactions treatment in the MTP construction both in terms of dispersion interactions [4] and electostatics [5]. Another recent methodological development is related to the use of the low-rank matrix and tensor factorization to compress radial parameters of MLIPs (polynomial models such as MTP and atomic cluster expansion [6] were used as examples) to perform calculations more efficiently [7]. The MLIP-4 package [8] contains these methodological developments.

In the application part, we will demonstrate how we used MTPs to efficiently model lattice thermal conductivity of structures with defects [9] and of the peculiar Moiré lattices of hydrogenated graphene and boron nitride [10]. We applied MTPs to model the physical properties of liquid molecular electrolytes and have shown that active learning can be used to collect a training set, with which it is possible to treat long-range interactions explicitly [11]. We will also show how learning on atomic environments can be used to parameterize MTPs, which are then used for large-scale simulations of the Cs diffusion in amorphous and polycrystalline SiC [12]. MTPs can be also used to speed up crystal structure prediction process, and we will demonstrate how we do it for pharmaceutically-relevant molecular crystals and crystalline inorganic non-linear optical semiconductors [13, 14]. Using the former case, we will also highlight the importance of the treatment of nuclear quantum effects [15] and the proper choice [16] of the exchange-correlation functional used in the data set preparation step once the calculations are done in the scope of density-functional theory.

2. Related works and Results

2.1 Methodological developments

The number of parameters in the basis sets of MLIP influences both the size of the training dataset required and the computational speed. Consequently, compressing MLIPs by reducing the number of parameters is a promising route to more efficient simulations. We used low-rank matrix and tensor factorizations under fixed-rank constraints to achieve this compression [7] and have shown that such compression (even by 50%) still allowed us to perform proper polymorph's ranking using glycine as example (see Fig. 1).

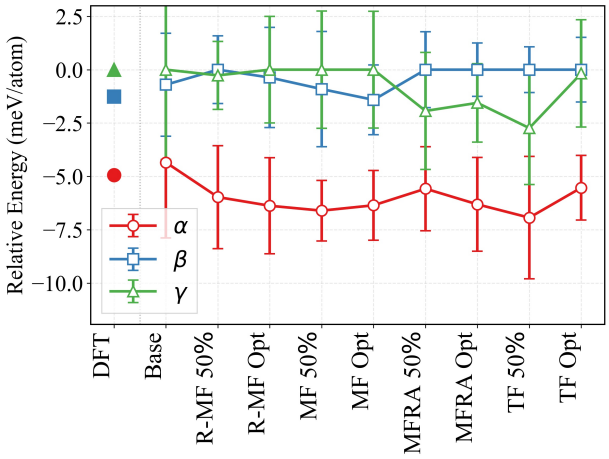

Fig. 1: Relative stability of glycine polymorphs calculated using MTP of the 20th level with different compression algorithms and DFT. Averaging is done over 10 separately trained potentials for each model. See details in work [7].

To incorporate electrostatics, fixed per-element point charges offer a simple baseline, while more transferable models learn environment-dependent charges from reference data, and globally dependent charges address non-local effects [5]. Our MTP-QRd model employs fixed charges per-element to test if explicit electrostatics improves the modeling of EC/EMC mixtures [11], where local MLIPs have previously sufficed.

2.2 Applications.

The diffusion mechanism of Cs in high energy grain boundaries (HEGBs) of silicon carbide (SiC) remained unsolved due to the lack of reliable and computationally efficient interatomic potentials. We used MTP to resolve this problem. Simulations shown that

Cs diffuses following a cage-breaking mechanism [12]. Such calculations were done by utilizing active learning on atomic environments methodology, which is sketched in Fig. 2.

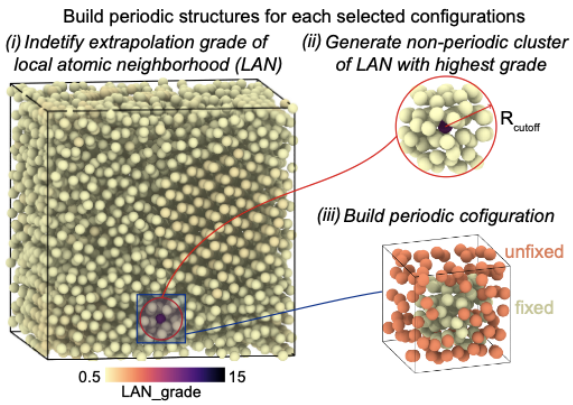

Fig. 2: Schematic representation of the learning on atomic environments procedure. See details in the work [12].

In the work [11], we demonstrated that active learning can automatically generate diverse training sets, enabling reliable molecular dynamics simulations of pure ethylene carbonate (EC), ethyl methyl carbonate (EMC), their mixtures, and $LiPF_6$ solutions. The resulting MTPs exhibit excellent transferability across various EC/EMC compositions, producing ionic conductivities within 11% mean deviations from experiments. In addition, we assessed the impact of explicitly incorporating electrostatics by extending MTP with a charge redistribution scheme. Our results show that this extended MTP achieves accuracy comparable to MTP for EC/EMC mixtures with fewer parameters and reproduces ionic conductivity with only a 6% mean deviation from experiment.

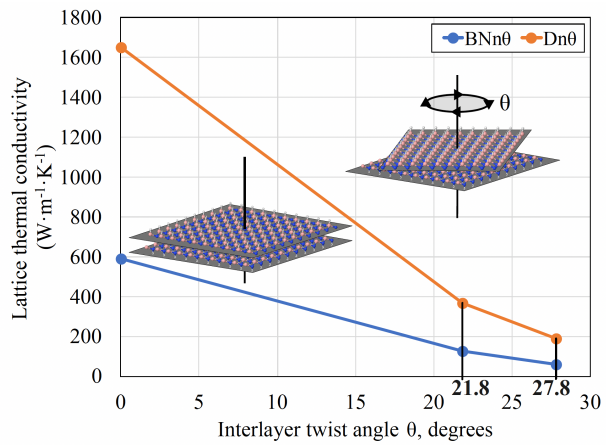

Fig. 3: Temperature dependence of the lattice thermal conductivity of the hydrogenated graphene and boron nitride.

In the works [10, 9] we have shown how MTPs can be used to effectively model temperature dependence of the lattice thermal conductivity (LTC) of complex compounds in the scope of Green-Kubo theory. In [9] we quantified the influence of different defects on the thermal conductivity of PbTe, whereas in [10] we evaluated LTC of complex Moiré lattices of the hydrogenated graphene and boron nitride. In the latter work it has been shown that anharmonic effects cause tremendous influence and should be taken into account to quantitatively estimate LTC of these compounds (see Fig. 3).

We are also going to discuss how path-integral molecular dynamics simulations can be performed with MTP [15] and how it can be used for proper molecular crystals structure prediction and ranking [13]. That said, we will also highlight how the proper DFT-based dataset should be constructed [16] for molecular crystals.

In summary, we are going to discuss recent methodological developments done with MTP model and recent applications where MTP showed its efficiency. In addition, we will discuss future work that should be done to generate MLIPs for more realistic matter simulations.

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