First-Principles Multiscale Modeling Enabled by Machine Learning Interatomic Potentials

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ABSTRACT SUBMISSION

In the conventional and everyday-life finite element (FE) simulations of engineering systems and products, prior to starting the calculations, materials and interactions properties are required to be provided as inputs to the models. On this basis, the development of accurate and robust theoretical approaches for elaborated examinations of various material properties, is highly advantageous in order to enhance the design process and minimize the necessity of complex experimental tests. Since the birth of the concept of machine learning interatomic potentials (MLIPs) in 2007 by Behler, and Parrinello [1], a growing interest has been developed to the replacement of empirical interatomic potentials (EIPs) with MLIPs, in order to conduct more accurate and reliable molecular dynamics calculations. As an exciting novel progress, recently the applications of MLIPs have been extended towards the exploration of the thermal transport and mechanical properties, providing novel opportunities not heretofore efficiently achievable, neither by EIPs nor by density functional theory (DFT) calculations. In this work, we first illustrate that how the combination of EIPs with FE multiscale simulations, could provide useful vision on the thermal and mechanical responses of nanostructured materials at the continuum level. Next, by considering several examples of recent studies, the robustness of MLIPs in the analysis of the mechanical and thermal properties will be discussed, and their superiority over EIPs and DFT methods will be emphasized. It will be finally highlighted that MLIPs furthermore offer astonishing capabilities to marry the robustness of DFT method with continuum mechanics, enabling the first-principles multiscale modeling of mechanical and thermal properties [2,3] of nanostructures at continuum level, with minimal prior physical knowledge, DFT level of accuracy and affordable computational costs.

METHODOLOGY

The first-principles multiscale modeling of mechanical and thermal conduction properties [2,3], comprises four major steps, which are schematically shown in Figure 1. In the first step, DFT simulations are carried out over stress-free and strained atomic configurations under varying temperatures to prepare required training datasets. Next, MLIPs are fitted using the two-step passive training approach [2,3]. To obtain the mechanical or thermal properties of pristine and heterostructure phases at room temperature, MLIP-based classical molecular dynamics calculations are employed. In the final step, on the basis of data provided by MLIP-based molecular dynamics simulations, the heat transport and/or mechanical responses of macroscopic heterostructures can be examined using the continuum FE method.

CONCLUSION

Machine learning interatomic potentials enabled first-principles multiscale modeling is believed to inherit an outstanding prospect to develop fully computerized platforms, to design and optimize novel materials and structures, with enhanced performances.

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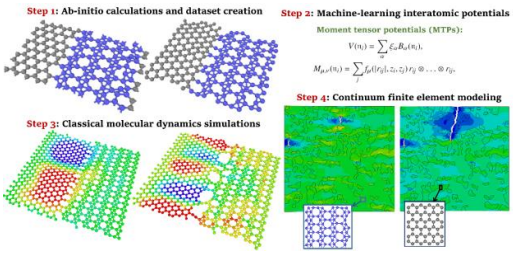

Fig. **1**. Main steps to conduct the first-principles multiscale modeling of mechanical properties (reprinted from [2], copyright 2021, John Wiley & Sons).