

## Accepted Manuscript

Accurate interatomic force field for molecular dynamics simulation by hybridizing classical and machine learning potentials

Peng Wang, Yecheng Shao, Hongtao Wang, Wei Yang

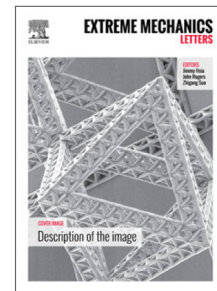
PII: S2352-4316(18)30159-7  
DOI: <https://doi.org/10.1016/j.eml.2018.08.002>  
Reference: EML 394

To appear in: *Extreme Mechanics Letters*

Received date: 10 July 2018  
Revised date: 14 August 2018  
Accepted date: 15 August 2018

Please cite this article as: Accurate interatomic force field for molecular dynamics simulation by hybridizing classical and machine learning potentials, *Extreme Mechanics Letters* (2018), <https://doi.org/10.1016/j.eml.2018.08.002>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.



# Accurate interatomic force field for molecular dynamics simulation by hybridizing classical and machine learning potentials

Peng Wang<sup>1,2</sup>, Yecheng Shao<sup>2,3</sup>, Hongtao Wang<sup>2,3\*</sup>, Wei Yang<sup>2,3\*</sup>

1 Materials Genome Institute, Shanghai University, Shanghai 200444, China

2 Center for X-mechanics, Zhejiang University, Hangzhou 310027, China

3 Institute of Applied Mechanics, Zhejiang University, Hangzhou 310027, China

## ABSTRACT

Full atom simulations have demonstrated the scalability for billions of atoms, but still suffered from the transferability of semi-empirical interatomic potentials. We propose a dynamic multiscale molecular dynamics (MD) simulation method with both high accuracy and efficiency in interatomic force field calculation by hybridizing both classical and machine learning (ML) potentials. A dynamic procedure has been adopted by evaluating the centro-symmetry parameter of evolving microstructures during MD simulations and accordingly modifying the highly distorted regions depicted by ML potentials. Atomic force field calculation in near-perfect or perfect lattices remain sticking to the fast EAM potential, which precisely captures the long range elastic interactions. A handshaking region is introduced in order to enforce the continuity in atomic interactions. The MD simulations using a dynamic multiscale scheme can achieve the *ab-initio* accuracy without raising considerable computational cost. The foundation of this approach deeply roots in the facts that the ML method has

---

\* To whom correspondence should be addressed. E-mail address: [htw@zju.edu.cn](mailto:htw@zju.edu.cn) (Hongtao Wang) and [yangw@zju.edu.cn](mailto:yangw@zju.edu.cn) (Wei Yang)

Download English Version:

<https://daneshyari.com/en/article/8954379>

Download Persian Version:

<https://daneshyari.com/article/8954379>

[Daneshyari.com](https://daneshyari.com)