Han Wang

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Educational Background & Employment

2021 –	**Professor**	Institute of Applied Physics and Computational Mathematics, Beijing, P.R. China
2015 – 2021	**Associate Professor**	Institute of Applied Physics and Computational Mathematics, Beijing, P.R. China
2014 – 2015	**Asistant Professor**	Institute of Applied Physics and Computational Mathematics, Beijing, P.R. China
2011 – 2014	**Postdoctoral Researcher**	Department of Mathematics & Computer Science, Freie Universität Berlin, Germany
2006 – 2011	**Ph.D. in Computational Math.**	School of Mathematical Sciences, Peking University, Beijing, P.R. China *Supervisor:* Prof. Pingwen Zhang
2007 – 2008	**Visiting Study**	Max-Planck Institute for Polymer Research, Mainz, Germany
2002 – 2006	**B.S. in Computational Math.**	School of Mathematical Sciences, Peking University, Beijing, P.R. China

Current Research Interests

Multiscale modeling and simulation.

Numerical analysis and fast algorithms for molecular dynamics.

Awards

ACM Gordon Bell Prize (2020).
Pushing the limit of molecular dynamics with ab initio accuracy to 100 million atoms with machine learning.
with Weile Jia, Mohan Chen, Denghui Lu, Lin Lin, Roberto Car, Weinan E and Linfeng Zhang

Selected Publications

1. Dongdong Wang, Yanze Wang, Junhan Chang, Linfeng Zhang*, Han Wang*, Weinan E
Efficient sampling of high-dimensional free energy landscapes using adaptive reinforced dynamics,
Nature Computational Science, **2**, 20-29 (2022).

2. Linfeng Zhang, Han Wang*, Roberto Car* and Weinan E,
The Phase Diagram of a Deep Potential Water Model ,
Physical Review Letters, **126**(23), 026704 (2012).

3. Yixiao Chen, Linfeng Zhang*, Han Wang*, and Weinan E
DeePKS: A Comprehensive Data-Driven Approach toward Chemically Accurate Density Functional The-

ory ,
Journal of Chemical Theory and Computation, **17**(1), 170–181 (2021).

4. Yuzhi Zhang, Haidi Wang, Weijie Chen, Jinzhe Zeng, Linfeng Zhang*, Han Wang*, Weinan E*
DP-GEN: A concurrent learning platform for the generation of reliable deep learning based potential energy models ,
Computer Physics Communications , **253**, 107206 (2020).

5. Linfeng Zhang, De-Ye Lin, Han Wang*, Roberto Car and Weinan E* Active learning of uniformly accurate interatomic potentials for materials simulation ,
Physical Review Materials , **3**, 023804 (2019).

6. Linfeng Zhang, Han Wang*, Weinan E*,
Reinforced dynamics for enhanced sampling in large atomic and molecular systems,
The Journal of Chemical Physics, **148**, 124113 (2018).

7. Han Wang*, Linfeng Zhang*, Jiequn Han, Weinan E,
DeePMD-kit: A deep learning package for many-body potential energy representation and molecular dynamics,
Computer Physics Communications, **228**, 178–184 (2018).

8. Linfeng Zhang, Jiequn Han, Han Wang*, Roberto Car, Weinan E*,
Deep Potential Molecular Dynamics: a scalable model with the accuracy of quantum mechanics,
Physics Review Letters, **120**, 143001 (2018).

9. Han Wang*, Xingyu Gao and Jun Fang
Multiple Staggered Mesh Ewald: Boosting the Accuracy of the Smooth Particle Mesh Ewald Method,
Journal of Chemical Theory and Computation, **12**(11), 5596-5608 (2016).

10. Han Wang* and Christof Schütte*,
Building Markov State Models for Periodically Driven Non-Equilibrium Systems,
Journal of Chemical Theory and Computing, **11**(4), 1819–1831 (2015).

11. Han Wang, Carsten Hartmann, Christof Schütte and Luigi Delle Site*,
Grand-canonical-like molecular-dynamics simulations by using an adaptive-resolution technique,
Physical Review X, **3**(1), 011018 (2013).

* To whom correspondence should be addressed.

Scientific Software

- DeePMD-kit, A deep learning package for many-body potential energy representation and molecular dynamics.
with Linfeng Zhang, Jiequn Han, Roberto Car, Weinan E and many contributors.

- DPGEN, The deep potential generator to generate a deep-learning based model of interatomic potential energy and force field.
with Yuzhi Zhang, Haidi Wang, Weijie Chen, Jinzhe Zeng, Linfeng Zhang, Weinan E and many contributors