Han Wang

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Educational Background & Employment

2014 –	**Research Scientist**	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

Employing deep learning techniques to address electronic structure problems.

Developing deep learning methods for modeling potential energy surfaces and their applications.

Utilizing deep learning methods for free energy modeling and enhanced sampling.

Software packages

DeePMD-kit	`https://github.com/deepmodeling/deepmd-kit`
DP-GEN	`https://github.com/deepmodeling/dpgen`
DP-GEN2	`https://github.com/deepmodeling/dpgen2`
dpdata	`https://github.com/deepmodeling/dpdata`

Selected Publications

1. 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).

2. 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).

3. 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).

4. 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).

5. Weile Jia, Han Wang, Mohan Chen, Denghui Lu, Lin Lin, Roberto Car, Weinan E and Linfeng Zhang,
   Pushing the limit of molecular dynamics with ab initio accuracy to 100 million atoms with machine learning,
   SC'20: Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis, **5**, 1-14 (2020).

6. Linfeng Zhang, Han Wang, Roberto Car and Weinan E,
   The Phase Diagram of a Deep Potential Water Model,
   Physical Review Letters, **126**, 236001 (2021).

7. 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 (2021).

8. Yixiao Chen, Linfeng Zhang, Han Wang, and Weinan E,
   DeePKS: A comprehensive data-driven approach toward chemically accurate density functional theory,
   Journal of Chemical Theory and Computation, **17**, 170–181 (2021).

9. Xiaoyang Wang, Yinan Wang, Linfeng Zhang, Fuzhi Dai and Han Wang,
   A tungsten deep neural-network potential for simulating mechanical property degradation under fusion service environment,
   Nuclear Fusion, **62**, 126013 (2022).

10. Duo Zhang, Hangrui Bi, Fu-Zhi Dai, Wanrun Jiang, Xinzijian Liu, Linfeng Zhang, Han Wang,
    Pretraining of attention-based deep learning potential model for molecular simulation,
    npj Computational Materials, **10**, 94 (2024).