

Towards Temperature-Dependent DeePMD Potential for Hydrogen Plasma

Onegin A.S.^{1,2,@} and Levashov P.R.^{1,2}

¹ Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow, 125412, Russia

² Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, 141701, Russia

@ onegin.as@phystech.edu

Path-integral Monte Carlo and other quantum simulation methods provide accurate descriptions of hydrogen plasma but are computationally prohibitive for large-scale or long-time simulations. In contrast, classical molecular dynamics (MD) is highly efficient yet relies on effective interaction models that often fail to capture essential quantum constraints. Machine learning potentials, such as DeepMD [1], offer a promising route to bridge this gap: by training on high-quality reference data, they can reproduce quantum-level accuracy at MD cost. In this work, we take key steps toward a DeepMD potential for hydrogen plasma, focusing on two critical physical ingredients: (i) explicit temperature dependence inherited from the underlying Kelbg pseudopotential [2, 3], and (ii) proper treatment of long-range Coulomb interactions via periodic Ewald summation. We show that omitting the latter leads to systematic errors, while its inclusion ensures physical consistency and stability. Training on data in the range $T = 24\text{--}97$ kK ($\Gamma = 0.1\text{--}0.5$) yields excellent accuracy: $R^2 = 0.967$ for energy and $R^2 = 0.987$ for forces, confirming the viability of machine-learned potentials for efficient, large-scale simulations of hydrogen plasma. The work was supported by the Russian Science Foundation grant 25-29-01649.

- [1] Wang H, Zhang L, Han J *et al.* 2018 *Computer Physics Communications* **228** 178–184
- [2] Kelbg G 1963 *Annalen der Physik* **467** 219–224
- [3] Filinov A V, Golubnychiy V O, Bonitz M, Ebeling W and Dufty J W 2004 *Phys. Rev. E* **70**(4) 046411 URL <https://link.aps.org/doi/10.1103/PhysRevE.70.046411>