Scilight

NEWS | FEBRUARY 24 2023

Deep neural network finds lack of transferability when modeling supercooled water FREE

Adam Liebendorfer

Scilight 2023, 081110 (2023)
https://doi.org/10.1063/10.0017466

AIP Publishing

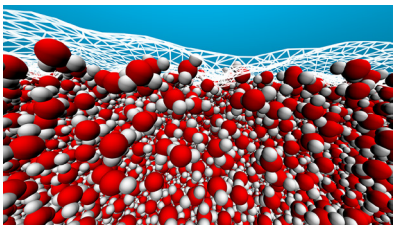
Scilight

24 February 2023

Deep neural network finds lack of transferability when modeling supercooled water

Adam Liebendorfer

Decomposition analyses of the molecular interactions show DNN potentials were unable to correctly represent fundamental individual many-body contributions.



Supercooled water continues to puzzle scientists as it freezes too quickly to be probed by experiments and moves too slowly to be modeled by high-level computer simulations. The emergence of machine learning has led to the development of deep neural network (DNN) potentials, which provide the energy of a molecular system given each atom's coordinates and can reproduce molecular energies and forces obtained by high-level but short computer simulations with high fidelity at a fraction of the computational cost.

Building upon recent machine learning developments, Zhai et al. have trained a DNN potential on their highly accurate, data-driven MB-pol potential to investigate the behavior of water from the boiling point to supercooled temperatures.

"While our DNN potentials enabled fast computer simulations that reproduced, nearly perfectly, the MB-pol results for supercooled water, their performance on other properties, such as vapor-liquid equilibrium properties, was far from satisfactory," said author Yaoguang Zhai.

To understand the lack of transferability of their DNN potentials, the authors performed thorough decomposition analyses of the molecular interactions, which demonstrated that the DNN potentials were unable to correctly represent individual many-body contributions.

When the authors improved the description of these individual many-body contributions, they found the performance of the DNN potentials on bulk properties had deteriorated, resulting in a "short blanket" dilemma as explained by author Alessandro Caruso.

"The lack of obvious transferability suggests that some caution should be used when exploring unknown thermodynamic states of a molecular system using DNN potentials," said author Sigbjørn Bore.

The authors hope their study will stoke further interest in new DNN architectures that can generalize across different phases and thermodynamic conditions.

Source: "A "short blanket" dilemma for a state-of-the-art neural network potential for water: Reproducing experimental properties or the physics of the underlying many-body interactions?," by Yaoguang Zhai, Alessandro Caruso, Sigbjørn Løland Bore, Zhishang Luo, and Francesco Paesani, *Journal of Chemical Physics* (2023). The article can be accessed at https://doi.org/10.1063/5.0142843.