Constructing High-dimension Neural Network Potentials for Oxide-Water Interfaces

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Oxide-water interfaces are promising systems for catalytic water splitting, a process of significant interest due to its potential in sustainable hydrogen production. Water molecules in the vicinity of the interface may spontaneously dissociate, resulting in a mixture of water, hydroxide ions and protons at the interface which dynamically interconvert via proton transfer reactions [1]. Understanding the detailed mechanisms of these proton transfer reactions and how they are affected by the morphology of the surface is an important step for improving the design of oxide-based catalysts. However, the complexity of the interface, which requires large simulation boxes to be treated in full detail, and the long time scales associated with dynamical processes present a substantial theoretical challenge for any method relying on explicit electronic structure calculations. High-Dimensional Neural Network Potentials (HDNNPs) [2] offer a solution to these challenges, enabling atomistic simulations with DFT-level accuracy at only a fraction of the computational expense. Here, we present the construction and application of a HDNNP suitable for studying various ZnO-water interfaces. Through molecular dynamics simulations with the HDNNP, we elucidate the impact of different surface facets on proton transfer reactions and long-range proton diffusion pathways.

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