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Machine-learning force fields for hydrogen and vacancy complex in tungsten

Tungsten (W) is used for plasma-facing components in nuclear fusion reactors, such as ITER and DEMO, due to its low tritium retention as well as its high melting point and low sputtering yields by hydrogen ions. However, experimental findings have shown that ambient deuterium (D) atoms in W can stabilize irradiation-induced defects, thereby enhancing D retention [1]. These results suggest that hydrogen-vacancy complexes may play a role in the stabilization of irradiation-induced defects. In this study, to understand hydrogen-vacancy (H-V) interaction microscopically, we developed a machine-learning force field (MLFF) for the H-V complexes in W based on density functional theory (DFT) calculations. In this MLFF, structural data (total energy, forces, and the stress tensor) were obtained from the DFT calculations using VASP [2], and local atomic environments were characterized by the Smooth Overlap of Atomic Positions (SOAP) descriptor [3]. Using Bayesian linear regression, unknown structural properties were predicted with quantified uncertainties. Then, the on-the-fly machine-learning approach was employed to efficiently sample training data to improve the MLFF. Using the MLFF, we calculated the binding energy of hydrogen atoms to a monovacancy and compared it with previous calculations of the DFT and model potentials [5,6]. For the vacancies containing one to eleven hydrogen atoms, the difference between DFT values and the predicted values by the present MLFF was 0.47eV at most, with the root mean squared error (RMSE) of 0.24eV. The agreement is significantly better than those of the model potentials [6], allowing MLFF-based MD simulations to achieve accuracy close to that of DFT calculations.

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