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Applying machine learning potential models to the study of hydrogen in metals: accurate property calculations, complex dynamics simulations, and challenges

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The transport and retention of hydrogen isotopes, deuterium and tritium, in materials affect the economics and sustainability of the fusion fuel cycle, as well as the integrity of materials due to the detrimental effects of hydrogen and helium produced by the alpha decay of tritium. Therefore, accurately predicting the behavior and effects of hydrogen in materials used as reactor components has been an important research topic in fusion engineering. However, the prediction is not a trivial task, mainly due to the complexity and diversity of hydrogen dynamics caused by lattice imperfections such as impurities, point defects, dislocations and grain boundaries, which limit the accuracy of experimental measurements. At the same time, the applicability of atomistic simulations has also been limited by a severe trade-off between computational accuracy and efficiency: to be specific, classical molecular dynamics (MD) is not accurate enough and density functional theory (DFT) calculations are not efficient enough.

Recently, the accuracy-efficiency tradeoff of atomistic simulations has been greatly improved by the advent and advanced implementation of machine learning potential models (MLIPs), which can achieve accuracy comparable to DFT calculations at much lower computational cost. In this presentation, focusing on hydrogen in metals, we will present our recent research progress and experience in the application of MLIPs, including (i) accurate calculations of fundamental properties, such as diffusivity, solubility, and permeability of hydrogen in metals, and (ii) calculations of kinetic parameters for complex surface processes to be used for rate models to simulate hydrogen behavior at the engineering scale. In addition, we will share our experiences in the construction and use of MLIPs, highlighting the challenges we have faced and what should be overcome to better utilize MLIPs for the study of hydrogen in metals.

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