Machine-learning interatomic potential development for studying tritium transport in breeders and breeder-blanket interfaces in fusion reactors

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Advancement in machine-learning interatomic potentials (MLIP) has allowed us to model complex material systems by training them on large datasets. Optimization of descriptors and implementation in graphical processing units has led to the use of MLIPs even for very large systems having millions of atoms. The bottleneck lies in the development of a comprehensive training dataset. Universal machine learning interatomic potential (UMLIP) foundation models and novel sampling techniques have been useful in efficiently building the training data. Yet, the robustness of the workflow and the performance of modern MLIPs remains unclear when it comes to complex material interfaces and materials under extreme environments.

In this talk, we discuss the development of MLIPs trained on density functional theory (DFT) and ab initio molecular dynamics (AIMD) data, to study the transport of tritium in fusion reactor breeder blanket systems. Understanding the retention and transport of tritium and accurately modelling it's inventory is crucial for the design of tritium breeder blankets. Specifically, we study tritium transport in liquid lithium-based breeders surrounded by vanadium structural material using two complementary MLIPs---an atomic cluster expansion (ACE) MLIP [1] and a neuroevolution potential (NEP) [2]---trained on comprehensive DFT datasets. We calculate the solubility and temperature-dependent diffusivity of hydrogen isotopes in the breeders and across the liquid-irradiated solid interface using molecular dynamics (MD). We also compare the performance of these MLIPs relative to a fine-tuned graphical atomic cluster expansion (GRACE) [3] UMLIP, both in terms of the required size of the training dataset and computational cost. We present an outlook on combining first principles and MD results with larger-scale modelling.

References:

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