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Interatomic potential development for H permeation in critical components

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A long-term prediction of hydrogen permeation in fusion-relevant materials requires the use of atomistic calculations with necessary details on microstructures, the accuracy of which is predominantly determined by the performance of interatomic potentials. The purpose of this study is to understand the available forms of potential models and develop a new set of potentials based on the best functional form. In this regard, our study is organized in two phases. In the first phase, we review potential models for various material systems, and next, we develop our own potentials for selected material systems.

In this talk, we will present the review of interatomic potentials used for the following material systems: (1) lithium oxide materials for breeder, (2) liquid metals for breeder, (3) SiC and composites for cladding, and (4) water as coolant.

The development status varies depending on the material systems, and interatomic potentials for lithium oxide materials in general are scarce, leaving breeder less exploited and hence making it a promising material system from developer's point of view. Nevertheless, validation and verification may be complicated for lithium oxide materials due to the complexity of lattice structures along with charge states.

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