

Technical Meeting on Nuclear Fusion Fuel Permeation in Reactor First Wall Components

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Interatomic potential development for H permeation in critical components

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In the first year of the coordinated research project, we have reviewed several material systems in which the impact of hydrogen permeation is crucial or critical ranging from first walls to functional materials to human tissues. Out of 9 materials systems reviewed, 4 systems have been selected for an in-depth study: (1) W/W alloys for a plasma-facing material, (2) Li-Ti-O ternary systems for a functional material, (3) bcc-Fe and ferrite for a structural material, and (4) concrete for a shielding material.

Different material systems are in different stages of development, e.g. W-H binary potentials are available but Li-Ti-O-H quaternary potentials are yet to be developed, and here we present a comparative study of different potentials where available, or a baseline set of first principles calculations where the relevant data are scarce. We discuss how we can balance the relative importance in the training set to minimize the reproducibility-transferability trade off.

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