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Unit mechanisms of interstitial He cluster diffusion in W: molecular and accelerated molecular dynamics simulations BLAS UBERUAGA, DANNY PEREZ, Los Alamos National Laboratory — Understanding unit mechanisms associated with He diffusion in W is critical for building physical models that are used for predicting performance of fusion energy systems. We use a combination of accelerated molecular dynamics (AMD) and conventional molecular dynamics (MD) to identify both the mechanisms and rates of migration for interstitial He clusters as a function of cluster size. AMD simulations reveal complex but definite mechanisms for diffusion of these clusters while MD shows that the migration mechanisms identified via AMD simulations dominate over a wide temperature range. Where there are deviations from a true Arrhenius behavior, we show that these can be explained by a super-basin effect in which a single pathway is still the bottleneck for leaving a complex arrangement of states that is sampled differently as a function of temperature. We discuss the implications for higher-level models of He evolution in W.

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