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Molecular Dynamics Analysis of Thermodynamic and Kinetic Properties of Surfaces and Interfaces of PdH_x

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ABSTRACT

This work uses molecular dynamics simulations to study surface and interface properties of PdH_x that are relevant to hydrogen storage applications. In particular, surface energies, interfacial energies, surface diffusivities, and surface segregations are all determined as a function of composition and temperature. During the course of the calculations, we demonstrated robust molecular dynamics methods that can result in highly converged finite temperature properties. Challenging examples include accurate calculations of hydrogen surface diffusivities that account for all possible atomic jump mechanisms, and constructions of surface segregation composition profiles that have negligible statistical errors. Our robust calculations reveal that the Arrhenius plots of hydrogen surface diffusion is ideally linear at low compositions, and becomes nonlinear at high compositions. The fundamental cause for this behaviour has been identified. This nonlinear surface diffusion behaviour is also in good agreement with available experimental data for bulk diffusion. The implication of our calculated properties on hydrogen storage application is discussed.

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