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Hydrogen on Nickel Surfaces at Elevated Temperatures LAUREN A. DILLON, ANGELO BONGIORNO, School of Chemistry and Biochemistry, Georgia Institute of Technology — Density functional theory, force fields, and Monte-Carlo simulations are used to address the adsorption, dissociation, and migration processes at elevated temperatures of hydrogen at nickel surfaces, which are key steps controlling the electrokinetics of conventional Ni-based anodes in solid-oxide fuel cells. In agreement with previous studies, this work shows that the adsorption and dissociation steps consist of (almost) barrierless processes, leading to the prompt formation of protons confined energetically to the superficial region. The bulk and surface diffusion of a proton in nickel is then addressed by using a multiscale approach. An effective interatomic potential describing the hydrogen-nickel interaction is first derived from density functional theory calculations. Then, molecular dynamics and Monte-Carlo simulations are combined to study in detail the hydrogen diffusion pathways and rates at increasing temperatures in the bulk and on the surface of Ni particles of various size. This work shows that the structural and thus energetic disorder at the surface increases for increasing temperatures, leading to the appearance of an anomalous surface diffusivity and to an increase of bulk migration pathways.

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