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Modeling Hydrogen-Metal Interactions

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Hydrogen-metal interaction attracts wide interests because it impacts a variety of material problems including hydrogen storage, hydrogen embrittlement, tritium science, and many more. Fundamental understanding of this interaction requires advanced computational methods to be combined with the state-of-the-art experimental characterization techniques. Such a combined approach can effectively elucidate adsorption/desorption of H_2 on metal surfaces, diffusion of hydrogen atoms inside materials., dynamic population of hydrogen atoms at various defective sites (e.g., dislocation cores, grain boundaries, and crack tips), and hydrogen effects on dislocation behavior and decohesion of interfaces. This presentation discusses our recent work that develops such modeling capabilities. First, we describe our effort to develop an Fe-Ni-Cr-H interatomic potential that is critically needed to enable fundamental modeling of widely used metal alloy for hydrogen application: stainless steel. We demonstrate how such a modeling capability can begin to enable understanding of the hydrogen embrittlemt problem from atomistic origins. Next, we present our Al-Cu-H bond order potential that can be used to study mechanical properties of a light weight metal alloy for hydrogen applications: Al-Cu alloys. We demonstrate how such a modeling apability can begine to enable understanding of hydrogen is incorpted into the materials from a molecular H_2 gas phase.

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