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Ab Initio Simulations of Hydrogen in Crystalline and Amorphous Metal Membranes WILLIAM HUHN, MIKE WIDOM, Carnegie Mellon University — Solid metallic membranes are used to separate hydrogen from other gases for clean energy applications. In order to create cheaper, more effective membranes for hydrogen separation, it is desirable to model hydrogen transport through the membrane. Amorphous metal membranes in particular have potential for this type of application due to low expense and high theoretical hydrogen capacity. We computationally model hydrogen absorption and transport through materials in order to find materials that can be used to construct effective membranes for hydrogen capture. In this talk, we will obtain hydrogen binding sites and diffusion barriers in order to model the hydrogen diffusion through various nickel-based amorphous alloys and compare them to associated crystalline structures as well as elemental palladium, which is favored for this application despite its high expense. Ab initio methods (specifically the Vienna Ab Initio Simulation Package, VASP) are used to develop the hydrogen binding energy spectrum, from which thermodynamic models can be constructed. Kinetic Monte Carlo methods are used to model the hydrogen transport through the bulk, from which we can obtain the permeability.

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