Kinetics of hydrogen transport in metal hydrides, crystalline alloys, and amorphous metals

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The diffusion of hydrogen is critical in the kinetics of hydrogen uptake and release in metal hydrides and in membrane-based approaches to hydrogen purification. First principles calculations have become a valuable counterpart to experimental methods to study hydrogen diffusion. Examples will be presented of using first principles calculations to understand hydrogen diffusion in a diverse range of solid materials, including metal hydrides in their bulk state and near interfaces, crystalline alloys for membrane applications, and amorphous metals for membrane applications.