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Using First-Principles Calculations to Describe Amorphous Metal Films for Hydrogen Purification
SHIQIANG HAO, MIKE WIDOM, DAVID SHOLL, GEORGIA INSTITUTE OF TECHNOLOGY TEAM, CARNEGIE MELLON UNIVERISTY TEAM — The increasing demand for clean and efficient energy has resulted in an increased global willingness to embrace the proposed hydrogen economy. The use of amorphous metal films as membranes to purify hydrogen has potential to overcome at least some of the disadvantages of existing crystalline metal membranes. We introduce a general strategy combining density functional theory and statistical mechanics to quantitatively predict solubility, diffusivity and permeability of interstitial H in amorphous metals. Our methods make it possible for the first time to quantitatively evaluate the performance of amorphous metal films as hydrogen purification membranes. These methods are introduced by examining amorphous Fe₃B and a crystalline analogue with the same composition. A membrane made from the amorphous material is predicted to have a hydrogen permeability 1.5-2 orders of magnitude higher than a crystalline membrane. The methods we introduce here will be useful in accelerating the development of amorphous membranes for practical applications.

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