Electronic Supplementary Material (ESI) for Energy & Environmental Science

Supporting Materials for Rapid Prediction of Hydrogen Permeation Through Amorphous metal Membranes: An Efficient Computational Screening Approach

Shiqiang Hao and David S. Sholl*

School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA 30332-0100, USA

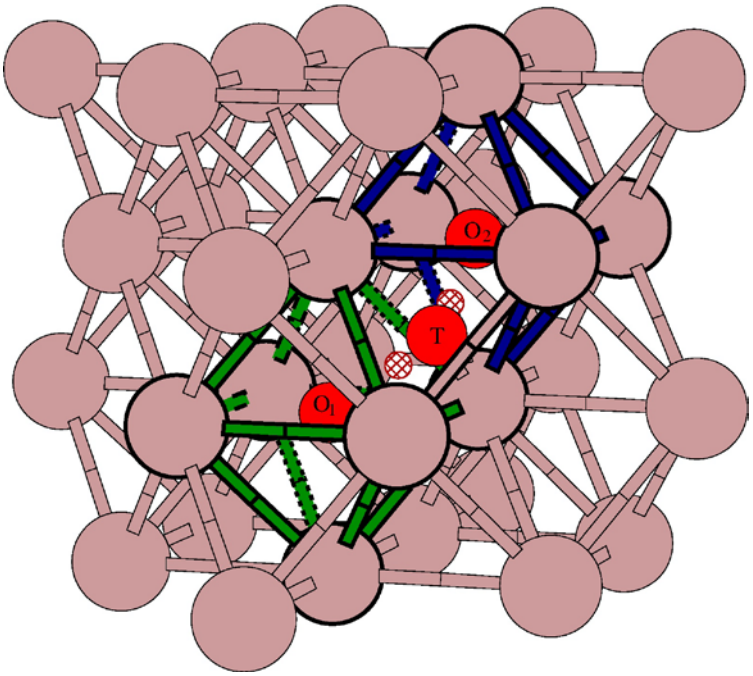

Figure S1. A schematic of the H diffusion mechanism in an FCC metal. A hydrogen atom (red ball) is initially located in an octahedral site (O_1) surrounded by green bars. By jumping over a transition state labeled as a small grid ball, the H atom gets to a neighboring tetrahedral site (T). The T-site hydrogen then jumps to another nearby octahedral site (O_2) surrounded by blue bars via a second transition state. A similar mechanism occurs in hops between neighboring interstitial sites in amorphous metals, although the geometry of the interstitial sites is less regular than in this example.

* Corresponding author. Email: david.sholl@chbe.gatech.edu

Table S1 Detailed DFT calculated and fitted solubility (at 600 K, 1 atm.) and diffusivity at corresponding H solubility. All values are normalized with the values for $Zr_{54}Cu_{46}$ at the same conditions.

	Solubility	Diffusivity
$Zr_{20}Cu_{80}$	0.78 (0.81)	0.47 (0.39)
$Zr_{54}Cu_{46}$	1.00 (1.07)	1.00 (1.21)
$Zr_{80}Cu_{20}$	1.76 (1.85)	0.56 (0.47)
$Zr_{40}Cu_{50}Ti_{10}$	1.17 (1.26)	1.45 (1.62)
$Zr_{50}Cu_{40}Ti_{10}$	1.26 (1.34)	2.02 (1.74)
$Zr_{70}Cu_{20}Ti_{10}$	1.84 (1.93)	0.89 (0.68)
$Zr_{10}Cu_{40}Ti_{50}$	1.22 (1.39)	0.84 (0.97)
$Zr_{25}Cu_{25}Ti_{50}$	1.53 (1.67)	0.61 (0.52)
$Zr_{40}Cu_{10}Ti_{50}$	2.09 (2.26)	0.33 (0.49)

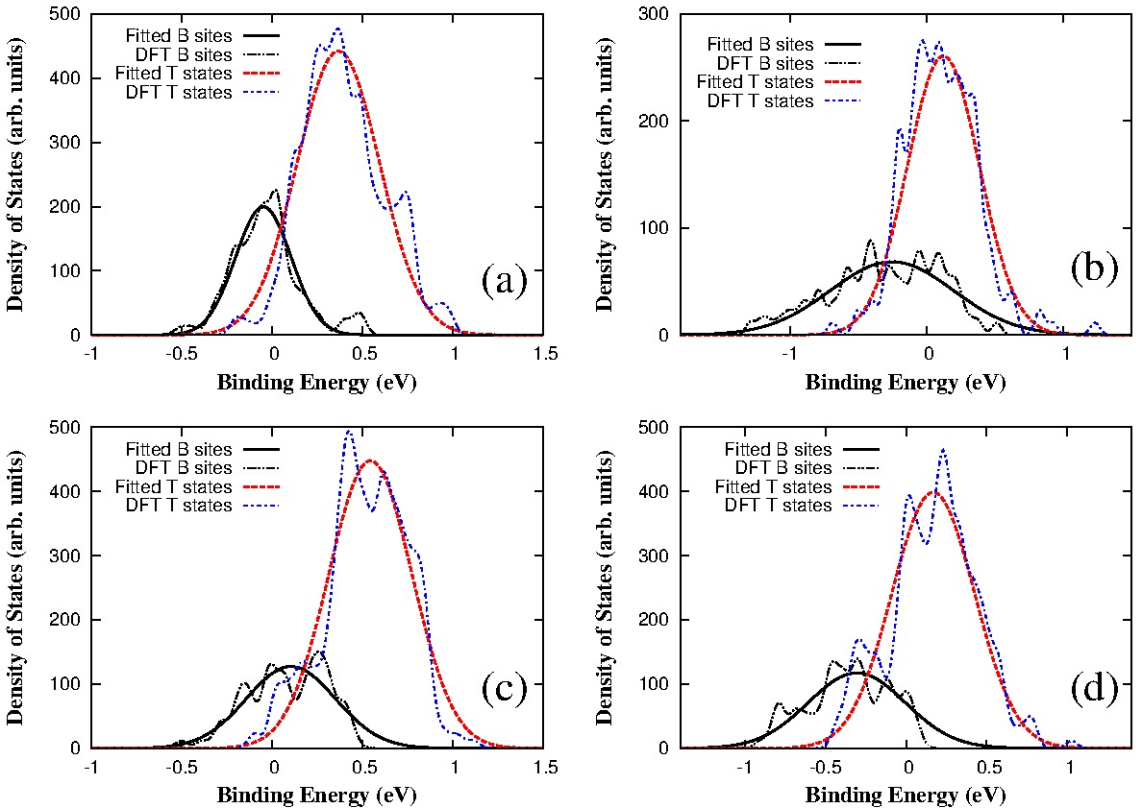

Figure S2. DFT and Gaussian model fitted binding energy and diffusion barrier distributions for (a) $Zr_{30}Cu_{60}Ru_{10}$, (b) $Zr_{30}Cu_{60}Rh_{10}$, (c) $Ta_{25}Ni_{60}Ti_{15}$, and (d) $Zr_{54}Cu_{46}$.