Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

First-Principles Study of Hydrogen Permeation in Palladium-Gold Alloys ANGELO BONGIORNO, SHUCHENG XU, School of Chemistry and Biochemistry, Georgia Instutute of Technology, Atlanta, GA 30332 — Density functional theory and lattice model calculations are combined to study the permeability of hydrogen in Pd lightly alloyed with Au. This study shows that small amounts of Au substitutions in Pd lead to, respectively, an increase and decrease of the diffusivity and solubility of hydrogen in the alloy. The competition between these two phenomena depends on temperature and can yield dilute PdAu membranes with a hydrogen permeability higher than pure Pd.

Angelo Bongiorno
School of Chemistry and Biochemistry,
Georgia Instutute of Technology, Atlanta, GA 30332

Date submitted: 26 Nov 2011 Electronic form version 1.4