Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Asymmetric Quantum Pd Films for Enhanced Hydrogen Separation[1] GUANGFEN WU, Southeast U, U of Tennessee-Knoxville, Oak Ridge National Laboratory, WENGUANG ZHU, U of Tennessee-Knoxville, Oak Ridge National Laboratory, JINLAN WANG, Southeast U, ZHENYU ZHANG, Oak Ridge National Laboratory, U of Tennessee-Knoville,U of Science and Technology of China — Based on density functional theory calculations and numerical simulations, we have investigated the permeation of H2 through ultra-thin Pd quantum films. The H2 flux can be highly increased by the elevation of the chemisorption-well on the permeate side without significantly blocking the subsurface-surface penetration. We find that Cu-coated asymmetric Pd quantum films (with the Cu monolayer on the permeate side) will enhance the capability for H2 separation: the recombination barrier for H is reduced from 1.36 to 0.79 eV, while the subsurface-surface penetration barrier is only slightly increased from 0.04 to 0.10 eV. Numerical simulations show enhanced H2 flux by 5 orders of magnitude as an upper-limit for asymmetric Pd films over symmetric ones under similar conditions.

[1]Supported by DMSE of USDOE, USNSF, and NNSF of China.

Guangfen Wu
Southeast U, U of Tennessee-Knoxville, Oak Ridge National Laboratory

Date submitted: 20 Dec 2010 Electronic form version 1.4