Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Hydrogen Embrittlement in Zirconium: a Quasi-Continuum Density Functional Theory Study[1] Q. PENG, Rensselaer Polytechnic Institute — The hydrogen embrittlement in Zirconium becomes a very important and emergent issue for academia, industry and policy makers as a result of the Japan nuclear accident. The hydride formation, diffusion and embrittlement in zircolay will impact dramatically on the development of advanced nuclear energy systems, the life time extension of the current nuclear fleet and dry storage of spent nuclear fuel. Quasi-Continuum Density Functional Theory (QCDFT) is a powerful concurrent multiscale method based entirely on density functional theory (DFT) and allows quantum simulations of materials properties of a large system with billions of atoms. Using QCDFT modeling, we found that the presents of hydrogen at the cracktip of zirconium, both on crack surface and in-bulk, will form zirconium hydrides and embrittle the system. The concentration of hydrogen and orientation of crack plays important roles in such embrittlement. The mechanism of hydrogen embrittlement under various loading conditions will be discussed.

[1]The authors would like to acknowledge the generous financial support from the Defense Threat Reduction Agency (DTRA) Grant # BRBAA08-C-2-0130, and the U.S. Nuclear Regulatory Commission Faculty Development Program under contract # NRC-38-08-950.

Q. Peng
Rensselaer Polytechnic Institute

Date submitted: 11 Nov 2011 Electronic form version 1.4