Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Glassy materials as a hydrogen storage medium[1] SEUNG-HOON JHI, Dept. of Physics, University of California at Berkeley and Chemical Science Division of Lawrence Berkeley National Lab., YOUNG-KYUN KWON, Dept. of Physics, University of California at Berkeley and University of Minnesota — The adsorption of molecular hydrogen on a glassy material and its relatives is studied with a use of pseudopotential density functional method. The binding energy and distance of adsorbed hydrogen is particularly calculated. It is found that the desorption temperature of hydrogen in layered boron oxide is significantly higher than that in carbon nanotubes as much as twice, which is attributed to heteropolar bonding in boron oxide. The effect of water addition to boron oxide on hydrogen adsorption is also investigated. Our results indicate that water may reduce the surface area of boron oxide but does little affect the hydrogen adsorption energy. We also calculated an optimum pore size for hydrogen diffusion into boron oxide. Current study demonstrates a pathway to the finding of a new class of materials for hydrogen storage media that can hold hydrogen at ambient conditions through physisorption.

[1]This work has been done at Nanomix, Inc.

Seung-Hoon Jhi
Dept. of Physics, University of California at Berkeley
and Chemical Science Division of Lawrence Berkeley National Lab.

Date submitted: 02 Dec 2004 Electronic form version 1.4