Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Determination of best models for adsorption of hydrogen in boron-doped carbon nanopores[1] RAINA CEPEL, MATTHEW BECKNER, CARLOS WEXLER, PETER PFEIFER, University of Missouri — Nanoporous carbon offers significant hydrogen storage capacities at low pressure and reversible conditions. Storage is achieved by physical adsorption of molecular hydrogen (H_2) on the surface of nanometer-size pores in the carbon matrix. Within the ALL-CRAFT collaboration (http://all-craft.missouri.edu), we conduct a proof-of-concept study of the prediction that boron-doped nanoporous carbon can store as much as 8 weight% at 47 bar and room temperature. By comparing theoretical and experimental H_2 adsorption isotherms for intrinsic and doped carbon, we determine which adsorption models and scenarios (e.g. localized vs. mobile) are consistent with experimental evidence.

[1]University of Missouri Research Board (RB-06-040), U.S. Department of Defense (N00164-07-P-1306), U.S. Department of Energy (DE-FG02-07ER46411)

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Date submitted: 03 Dec 2007 Electronic form version 1.4