MAR06-2005-003556

Abstract for an Invited Paper
for the MAR06 Meeting of
the American Physical Society

The potential of hydrogen storage in hydrate and graphitic systems

JOHN TSE, University of Saskatchewan

Many methods have been proposed for efficient storage of molecularhydrogen for fuel cell applications. Recently, it was found that molecular hydrogen can be stored in large quantity approaching the U.S. Department of Energy goals of6.5% mass ratio in ice clathrate under high pressure and low temperature [1]. Attempts were made to increase the stability of the clathrate. Unfortunately, so far the modified hydrates failed to meet the elusive goal [2,3]. To understand the thermodynamic stability and storage capacity, hydrogen occupancy in clathrate hydrate was examined with a statisticalmechanical model in conjunction with first-principles quantumchemistry calculations [4]. The theoretical approach is extended to graphitic systems [5]. It is shown that insufficiently accurate carbon–H_2 interaction potentials, together with the neglectand incomplete treatment of the quantum effects in previoustheoretical investigations led to incorrect conclusions forthe absorption capacity. A proper account of the contributionof quantum effects to the free energy and the equilibrium constantfor hydrogen adsorption suggest that the U.S. Department ofEnergy specification can be approached in a graphite-based physisorptionsystem. [1] W.L. Mao, H.-K. Mao, A.F. Goncharov, V.V. Struzhkin,Q Guo, Q., *et al. Science* 297, 2247–2249 (2002) [2] H. Lee, J. Lee, D.Y. Kim, J. Park, Y. Seo, H. Zeng, I.L. Moudrakovski, C.I. Ratcliffe, J.A. Ripmeester, *Nature* 434, 743-746, (2005) [3] L.J. Florusse, C.J. Peters, J. Schoonman, K.C. Hester, C.A. Koh, S.F. Dec, K.N. Marsh, E. D. Sloan, *Science*, 306, 469 – 471 (2004) [4] S. Patchkovskii, J.S. Tse, *Proc. Nat. Acad. Sci.*, 100, 14645-14650 (2003) [5] S. Patchkovskii, J.S. Tse, S.N. Yurchenko, L. Zhechkov, T. Heine, G. Seifert, *Proc. Nat. Acad. Sci.*, 102, 10439-10444 (2005)