INTERNATIONAL JOURNAL OF HYDROGEN ENERGY 35 (2010) 12864–12869

Available at www.sciencedirect.com

ScienceDirect

journal homepage: www.elsevier.com/locate/he

High density hydrogen storage in nanocavities: Role of the electrostatic interaction

L. Reguera [a,b], J. Roque [a], J. Hernández [a,c], E. Reguera [a,d,*]

[a] Centro de Investigación en Ciencia Aplicada y Tecnología Avanzada del IPN, Legaria 694, México D.F, Mexico
[b] Facultad de Química, Universidad de La Habana, La Habana, Cuba
[c] Universidad de Pinar del Río, Pinar del Río, Cuba
[d] Instituto de Ciencia y Tecnología de Materiales, Universidad de La Habana, La Habana, Cuba

ARTICLE INFO

Article history:
Received 4 August 2010
Received in revised form
2 September 2010
Accepted 2 September 2010
Available online 28 September 2010

Keywords:
Hydrogen storage
Hydrogen adsorption
Adsorption forces
Porous solids

ABSTRACT

High pressure H_2 adsorption isotherms at N_2 liquid temperature were recorded for the series of cubic nitroprussides, $Ni_{1-x}Co_x[Fe(CN)_5NO]$ with $x = 0, 0.5, 0.7, 1$. The obtained data were interpreted according to the effective polarizing power for the metal found at the surface of the cavity. The cavity volume where the hydrogen molecules are accumulated was estimated from the amount of water molecules that are occupying that available space in the as-synthesized solids considering a water density of 1 g/cm^3. The calculated cavity volume was then used to obtain the density of H_2 storage in the cavity. For the Ni-containing material the highest storage density was obtained, in a cavity volume of 448.5 Å^3 up to 10.4 hydrogen molecules are accumulated, for a local density of 77.6 g/L, above the density value corresponding to liquid hydrogen (71 g/L). Such high value of local density was interpreted as related to the electrostatic contribution to the adsorption potential for the hydrogen molecule within the cavity.

1. Introduction

The world economy formed in the last century is mainly based on the use of fossil fuels as energy source but, such development is untenable because the limited availability of these non-renewable resources and leads to an irreversible environmental catastrophe. The combustion of fossil fuels and their derivates produces the emission of large amounts of carbon dioxide which is responsible for the global warming and related climate changes [1]. From these facts, the idea of an economy based on hydrogen as energy bearer has emerged and consolidated in the last decades [1–3]. The hydrogen oxidation liberates 286 kJ/mol, three times the value obtained from gasoline, and produces an environmental friendly byproduct, water. The main challenge to have an energetic technology based on hydrogen as secondary energy bearer instead fossil fuels derivates, is probably the non-availability, up to date, of an appropriate hydrogen storage method. Hydrogen is a molecule of very low critical temperature (32.97 K) to be storage in liquid state for massive technological applications. Such feature of hydrogen also explains the difficulties found for its storage in high pressure vessels. From these facts, several alternative storage routes are being evaluated, among them the hydride formation in light weight materials [4,5], H_2 sequestering in molecular cages (clathrates) [6], and H_2 adsorption in solids of extended surface, mainly nanoporous materials [7,8]. This last method is particularly attractive because of its reversibility, a required feature of any viable H_2 storage technology.

The hydrogen molecule can be adsorbed through three types of adsorption forces [9]: 1) dispersive interactions, whose strength depends on the surface electron density, 2)

* *Corresponding author*. Instituto de Ciencia y Tecnología de Materiales, Universidad de La Habana, La Habana, Cuba.
E-mail address: ereguera@yahoo.com (E. Reguera).
0360-3199/$ – see front matter © 2010 Professor T. Nejat Veziroglu. Published by Elsevier Ltd. All rights reserved.
doi:10.1016/j.ijhydene.2010.09.007