



ELSEVIER

Contents lists available at ScienceDirect

Chemical Data Collections

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

Data Article

Hydrogen adsorption on surfaces with different binding energies



Lucyna Firlej^{a,d}, Justyna Rogacka^b, Katarzyna Walczak^a,
Bogdan Kuchta^{b,c,*}

^a Laboratoire Charles Coulombs, Université Montpellier 2, 34095 Montpellier, France

^b Department of Chemistry, Group of Chemical and Biochemical Processes, Wrocław University of Technology, Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland

^c Laboratoire MADIREL, Université Aix-Marseille-CNRS UMR 7246, 13396 Marseille, France

^d Department of Physics and Astronomy, University of Missouri, Columbia, MO 65211, USA

ARTICLE INFO

Article history:

Received 8 December 2015

Accepted 26 February 2016

Available online 9 March 2016

Keywords:

Hydrogen adsorption

Hydrogen storage

Energy of adsorption

ABSTRACT

The isotherms of molecular hydrogen adsorption in slit pores have been calculated at room temperature ($T = 298$ K) for various pore sizes, from 0.6 nm to 2.5 nm. The pressure has been varied from 0 to 120 bar (12 MPa). The wall surface has been characterized by different values of the adsorption energy, from 3 to 25 kJ/mol. The provided raw data give the number of molecules adsorbed per nm² of the adsorbing wall, and can be used for fast storage capacity screening of new porous adsorbents with known enthalpy of adsorption. The data are supplied with this article.

© 2016 Elsevier B.V. All rights reserved.

Specifications table

Subject area	Computational Chemistry, Physical Chemistry, Chemical Engineering, etc.
Compounds	Dihydrogen H ₂
Data category	Computational simulations
Data acquisition format	Isotherms
Data type	Simulated
Procedure	Monte Carlo simulations (grand canonical)
Data accessibility	With this article

* Corresponding author at: Laboratoire MADIREL, Université Aix-Marseille, 13396 Marseille, France. Tel.: +33 643551646.

E-mail address: bogdan.kuchta@univ-amu.fr, bogdan.kuchta54@gmail.com (B. Kuchta).

1. Rationale

Efficient and save storage of hydrogen for mobile applications (hydrogen fuel cell vehicles) remains the bottle-neck and one of the main challenges in hydrogen-based technologies. Among different storage methods, physical adsorption of molecular hydrogen in various porous structures is considered as the most attractive option: as the process of physisorption is reversible, the recovery of adsorbed hydrogen will be relatively easy. However, despite of more than 15 years of research [1,2] no material possesses yet the required adsorbing properties, and providing at least 75 g of H₂ per kg and 70 g per L of storing system [3–12]. An important research effort is still needed, to synthesize a material with required properties. In this paper we present a database of hydrogen adsorption model isotherms in slit pores with wall surfaces characterized by different binding energies. The model of slit pore gives a good estimation of the hydrogen uptake in carbon based materials [2–6]. The adsorption information is presented in a ready-to use form for future rapid screening of new porous structure from the point of view of potential hydrogen storage application. The only information required to estimate the total uptake is the enthalpy of hydrogen adsorption and pore size distribution.

The data base has been prepared using a homemade grand canonical Monte Carlo program, tested and verified for many years in our previous research projects [3–5], and the results were compared with the Material Studio Sorption [13] calculations.

Although it is still impossible to predict from numerical simulations how an optimal gas adsorbent should look like, computer modeling methods can partially help answer this question [14–17]. Two parameters have the essential influence on the gas uptake in a porous structure. The first one is the binding energy E_a between adsorbed hydrogen molecule and the adsorbing surface. Numerical modeling can provide very accurate information on the effect of this parameter on the total uptake. The second parameter is the specific surface area accessible for adsorption [17]. Usually both parameters are estimated during the initial experimental characterization of porous structures (for example, from nitrogen adsorption isotherms and calorimetric studies). If more structural information is available, in particular the pore size distribution, the final uptake can be calculated with higher accuracy. The ensemble of simulated isotherms published here will allow one to estimate whether a structure can be considered as potentially applicable new hydrogen sorbent.

2. Procedure

Among many models of the H₂–H₂ interaction exhaustively applied in the literature, we have chosen here a model that considers the H₂ molecules as structureless superatoms, interacting via Lennard–Jones (6–12) potential. The most practical model of H₂ superatoms interaction with graphene-like surface is the analytical form proposed by Steele [14]. In this model, a H₂ molecule interacts with carbon atoms in graphene through 6–12 potential energy; the energy of adsorbed particle is an integral over the whole graphene sheet, and depends only on the vertical distance of H₂ superatom from the surface (smooth surface approximation). The atomic corrugation of the pore wall can be taken into account by adding modulating corrugation term. However, the corrugation component is not explicitly treated in this paper as it represents a marginal fraction of the H₂–wall interaction energy (less than 1%). In this paper we present the detailed database of H₂ adsorption isotherms ($T = 298$ K) calculated for the binding energies of hydrogen molecule adsorbed on a surface in the range from 3 kJ/mol up to 25 kJ/mol. This covers the energies of weak hydrogen adsorbent (3 kJ/mol), typical activated carbons (4–6 kJ/mol) and the higher energies required for future applications [18]. The pore width is defined as the distance between the centers of atoms in the adjacent pore walls.

The information included in the isotherms is much more detailed than the results published before [3,12,17]. First of all, it covers the whole range of prospected working pressures of hydrogen storing vessels (0–120 bar), and the wide range of pores sizes, between 0.6 nm and 2.5 nm. This pore size range is necessary to accurately tailor the structure of the efficient hydrogen sorbent because only a monolayer of hydrogen can be adsorbed at any surface at ambient temperature. Furthermore, the prepared data base can be applied to analyze materials with heterogeneous surfaces, for which a distribution of binding energies must be assumed. Recently, we applied such procedure for reproducing

Download English Version:

<https://daneshyari.com/en/article/1180093>

Download Persian Version:

<https://daneshyari.com/article/1180093>

[Daneshyari.com](https://daneshyari.com)