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Materials for Hydrogen Storage in Nanocavities: Design criteria

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ABSTRACT

The adsorption potential for a given adsorbate depends of both, material surface and adsorbate properties. In this contribution the possible guest-host interactions for H_2 within a cavity or on a surface are discussed considering the molecule physical properties. Five different interactions contribute to the adsorption forces for this molecule: 1) quadrupole moment interaction with the local electric field gradient; 1) electron cloud polarization by a charge center; 3) dispersive forces (van der Waals); 4) quadrupole moment versus quadrupole moment between neighboring H_2 molecules, and, 5) H_2 coordination to a metal center. The relative importance of these five interactions for the hydrogen storage in nanocavities is discussed from experimental evidences in order to extract materials design criteria for molecular hydrogen storage.

1. Introduction

Hydrogen, because of its large heat combustion, 287 kJ/mole, and environmentally compatible byproduct, water, is being considered as an alternative to fossil fuel derivatives for mobile applications. However, molecular hydrogen has a low critical temperature (32.97 K) to be handled in liquid state for practical applications as fuel. Thereby, one of the challenges for the development of an energetic technology based on hydrogen is the availability of an appropriate method for hydrogen storage. One of the options that are being studied in that sense is its storage in nanocavities of light weight materials through physical interactions [21,26]. The physical interactions guarantee the process reversibility, a requirement for the storage process. Two merit figures appear as relevant for H_2 storage in porous solids for such applications: a gravimetric density in the 6–9 % range [3] and adsorption heats (ΔH_{ads}) in the 20–30 kJ/mole range [1,25]; this last one in order to maintain the hydrogen molecule as adsorbed species close to atmospheric conditions (298 K and 1 atm.). The target of 6–9 % of H_2 adsorbed is oriented to be able the combustible storage in a reasonable volume and weight of the host solid for a given vehicle autonomy. Up to date practically all the reported results on the hydrogen storage in porous solids remain short respect to these targets, which suggests that more basic studies and better materials design are required. A survey of the available literature on the H_2 adsorption in porous materials provides abundant information on the corresponding adsorption energy [17,21]. These energy values can be correlated with the nature of the involved guest-host interactions in order to obtain criteria for materials design. In this contribution the possible guest-host interactions for the hydrogen molecule within a nanocavity or on a solid surface are considered and the related stabilization energy discussed.

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