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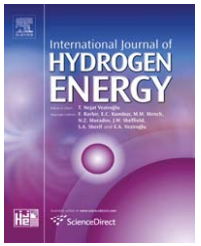

Materials for Hydrogen Storage in Nanocavities: Design criteria

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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.