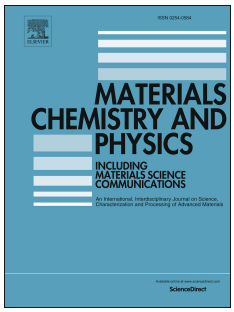
Accepted Manuscript



3-Dimensional nanopores on monolayer graphene for hydrogen storage

Xin Zhang, Shiwei Cao, Ning Zhang, Lei Wang, Ximeng Chen, Zhan Li

PII: S0254-0584(17)31038-6

DOI: 10.1016/j.matchemphys.2017.12.082

Reference: MAC 20264

To appear in: *Materials Chemistry and Physics*

Received Date: 22 June 2017

Revised Date: 28 October 2017

Accepted Date: 28 December 2017

Please cite this article as: X. Zhang, S. Cao, N. Zhang, L. Wang, X. Chen, Z. Li, 3-Dimensional nanopores on monolayer graphene for hydrogen storage, *Materials Chemistry and Physics* (2018), doi: 10.1016/j.matchemphys.2017.12.082.

3-Dimensional Nanopores on Monolayer Graphene for Hydrogen Storage☆

Zhang Xin[a,b,c], Cao Shiwei[b], Zhang Ning[a], Wang Lei[1], Chen Ximeng[a,*], Li Zhan[d,*]

[a] *The School of Nuclear Science and Technology, Lanzhou University, Lanzhou, 730000, P.R. China.*
[b] *Institute of Modern Physics, Chinese Academy of Sciences, Lanzhou, 730000, P.R. China.*
[c] *College of Chemistry, Sichuan University, Chengdu, 610065, P.R. China.*
[d] *Lanzhou Institute of Chemical Physics, Chinese Academy of Sciences, Lanzhou, 730000, P.R. China.*

Abstract

Hydrogen storage in solids is becoming an ever more important technology. We theoretically design a completely new material for hydrogen storage, which is quite different from the present materials. This kind of material, base on monolayer graphene, is thought to be extremely flexible. First-principles calculations and kinetic theory of gases are employed to evaluate this material. The results demonstrate that it is promising for hydrogen storage. More than anything, the hydrogen storage capacity of this material is about $4\,\mathrm{mmol\,g^{-1}}$ at 300 K and 1 atm.

1. Introduction

Hydrogen, widely discussed in the context of energy, has been recognized as a possible future carrier of energy on an economy-wide scale. However, one of the challenges that need to be overcome before the hydrogen economy

☆Supplementary data: Front and side elevation of nanocaves. ADCH charge analyses and electron densities of the nanocaves. Hydrogen molecules diffusion behavior in the nanocaves (investigated by using first principles molecule dynamics calculations).

*Corresponding author

Email addresses: chenxm@lzu.edu.cn. (Chen Ximeng), lizhancg@licp.cas.cn (Li Zhan)