

Accepted Manuscript

Article

Molecular sieving through a graphene nanopore: non-equilibrium molecular dynamics simulation

Chengzhen Sun, Bofeng Bai

PII: S2095-9273(17)30127-5
DOI: <http://dx.doi.org/10.1016/j.scib.2017.03.004>
Reference: SCIB 79

To appear in: *Science Bulletin*

Received Date: 11 January 2017
Revised Date: 22 February 2017
Accepted Date: 28 February 2017

Please cite this article as: C. Sun, B. Bai, Molecular sieving through a graphene nanopore: non-equilibrium molecular dynamics simulation, *Science Bulletin* (2017), doi: <http://dx.doi.org/10.1016/j.scib.2017.03.004>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.



Article

Received 11 January 2017, Revised 22 February 2017, Accepted 28 February 2017

**Molecular sieving through a graphene nanopore: non-equilibrium
molecular dynamics simulation**

Chengzhen Sun, Bofeng Bai*

State Key Laboratory of Multiphase Flow in Power Engineering, Xi'an Jiaotong University,
Xi'an 710049, China

*Corresponding author. E-mail: bfbai@mail.xjtu.edu.cn

Abstract

Two-dimensional graphene nanopores have shown great promise as ultra-permeable molecular sieves based on their size-sieving effects. We design a nitrogen/hydrogen modified graphene nanopore and conduct a transient non-equilibrium molecular dynamics simulation on its molecular sieving effects. The distinct time-varying molecular crossing numbers show that this special nanopore can efficiently sieve CO₂ and H₂S molecules from CH₄ molecules with high selectivity. By analyzing the molecular structure and pore functionalization-related molecular orientation and permeable zone in the nanopore, density distribution in the molecular adsorption layer on the graphene surface, as well as other features, the molecular sieving mechanisms of graphene nanopores are revealed. Finally, some implications on the design of highly-efficient graphene nanopores, especially for determining the porosity and chemical functionalization, as gas separation membranes are summarized based on the identified phenomena and mechanisms.

Keywords: Graphene Nanopore, Molecular Sieve, Molecular Dynamics, Gas Separation Membrane

1. Introduction

Graphene and its derivatives [1-4] are reasonably thought to be very promising candidates for separation membrane materials owing to their atomic thickness. With

Download English Version:

<https://daneshyari.com/en/article/5788782>

Download Persian Version:

<https://daneshyari.com/article/5788782>

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