Article

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Chengzhen Sun, Bofeng Bai

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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 CO_2 and H_2S molecules from CH_4 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