Selective permeability of biphenylene carbon (BPC) membrane: performance in CO₂/H₂ gas separation

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Abstract

Biphenylene carbon is a porous carbon allotrope with a thickness of a single atom. An open question is whether the BPC natural porosity can be exploited to create selective permeable membranes. We have carried out full atomistic Molecular Dynamics simulations to show that BPC is highly selective for H₂. We have also investigated its possible application for H₂ purification.

Key words:

Biphenylene carbon (BPC), gas separation, selectively permeable membrane

Introduction

The recent discovery of new nanomaterials has already resulted in effective new applications. Among these new materials, graphene¹, a “two-dimensional” carbon structure with a single atom thickness, has been exploited in numerous technological applications, including selective membranes. It was recently demonstrated that graphene is impermeable to standard gases².

In part due to graphene impermeability, there is a renewed interest in other carbon-based structures. One example is biphenylene carbon (BPC), which is a porous carbon allotrope and, like graphene, has a thickness of a single atom³. The BPC pores are regular decagons with a diameter of 3.2 Å.

An open question is whether the BPC natural porosity can be exploited to create selective permeable membranes, which could lead to promising technological applications, such as gas separation. In this work, we have investigated the BPC permeability and selectivity to CO₂ and H₂ gases.

Figure 1. BPC molecular geometry.

Results and Discussion

Fully atomistic Molecular Dynamics⁴ (MD) simulations were performed to predict the gas adsorption and permeability to single H₂ and CO₂ components. The simulation system consists of a single BPC sheet into contact with a gas reservoir under different pressure values. The separation mechanism of the binary CO₂/H₂ mixture was also evaluated.

(a)

Figure 2. (a) BPC permeability for single H₂ and CO₂ gases; (b) Density profile for single H₂ and CO₂ gas adsorption through BPC membrane; (c) MD snapshots of the CO₂/H₂ mixture system at the beginning and at the end of the simulation; (d) H₂/CO₂ BPC selectivity for CO₂/H₂ mixture.

Our results show that BPC can exhibit selective permeability (and high selectivity for H₂) depending on the external pressure values.

Conclusions

We have carried out full atomistic MD simulations to predict BPC permeability for H₂ and CO₂ and, also, to evaluate BPC selectivity for H₂ and CO₂ mixture. Our results show that BPC is highly selective for H₂, with good potential to work as a molecular sieve for H₂ purification.

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