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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 wheter 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, graphene[1], 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 gases[2].

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 atom[3]. The BPC pores are regular decagons with a dimeter 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 CO_2 and H_2 gases.

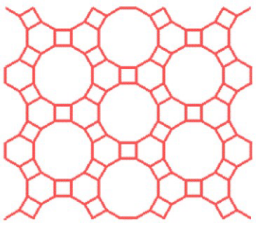
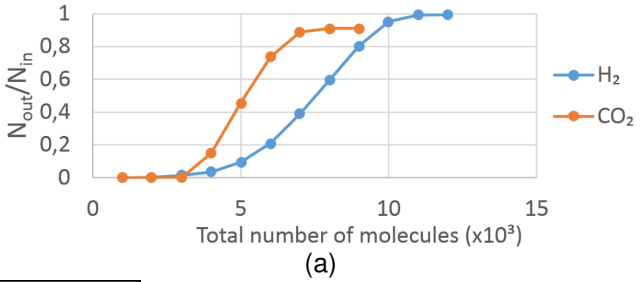


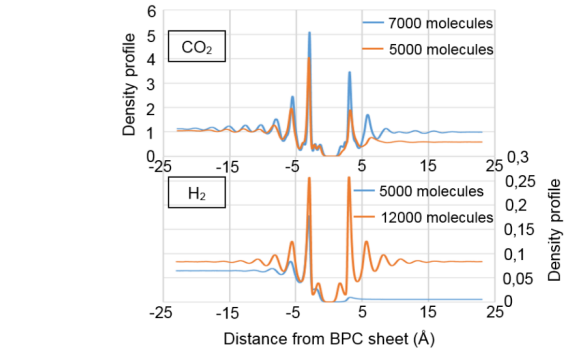
Figure 1. BPC molecular geometry.

Results and Discussion

Fully atomistic Molecular Dynamics[4] (MD) simulations were performed to predict the gas adsorption and permeability to single H_2 and CO_2 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 CO_2/H_2 mixture was also evaluated.



(a)



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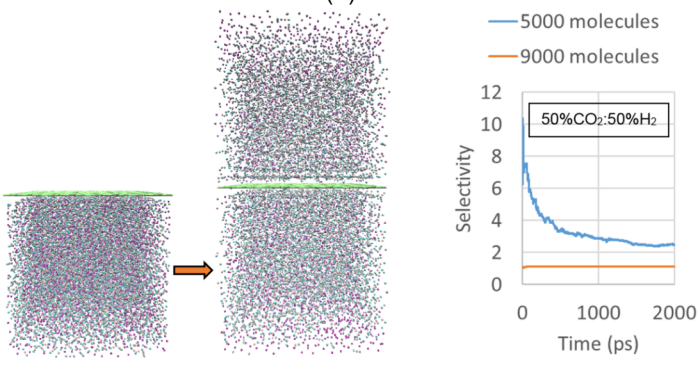

(c) (d)

Figure 2. (a) BPC permeability for single H_2 and CO_2 gases; (b) Density profile for single H_2 and CO_2 gas adsorption through BPC membrane; (c) MD snapshots of the CO_2/H_2 mixture system at the beginning and at the end of the simulation; (d) H_2/CO_2 BPC selectivity for CO_2/H_2 mixture.

Our results show that BPC can exhibit selective permeability (and high selectivity for H_2) depending on the external pressure values.

Conclusions

We have carried out full atomistic MD simulations to predict BPC permeability for H_2 and CO_2 and, also, to evaluate BPC selectivity for H_2 and CO_2 mixture. Our results show that BPC is highly selective for H_2, with good potential to work as a molecular sieve for H_2 purification.

Acknowledgement

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