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, graphene, 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. 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. 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.

Results and Discussion
Fully atomistic Molecular Dynamics (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.

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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