Impermeability properties of Biphenylene Carbon (BPC) membranes

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Abstract
Biphenylene carbon (BPC) is a graphene-like porous carbon allotrope. Due to its 2D topology and single atom thickness (planar sheet), BPC can, in principle, work as a membrane impermeable to gases. In this work, through fully atomistic molecular dynamics simulations we show that BPC membranes are indeed impermeable to oxygen, argon and carbon dioxide molecules.

Key words:
Biphenylene permeability/impermeability, biphenylene nanoresonator, Molecular Dynamics.

Introduction
In the past few years, the large amount of theoretical and experimental work on graphene1 (a single graphite layer) provided a better understanding of its properties. In addition to unique electronic properties, graphene has also exceptional mechanical properties, which has been exploited in many technological applications, as in the case of nanoresonators. In fact, it was recently demonstrated2 that graphene, due its bidimensional feature and single atom thickness, can work as a membrane impermeable to gases, as argon and helium.

There are other pure carbon bidimensional structures such as graphynes3 and biphenylene carbon (BPC) (Figure 1)4. In this work we investigated whether biphenylene, which is a graphene-like porous carbon membrane, can also work as an impermeable membrane or exhibit some selective permeability.

Results and Discussion
An initial approach to estimate the BPC permeability is to calculate the potential barrier provided by the membrane when a gas molecule pass through one of its pores (Figure 2). These estimations were obtained through fully atomistic molecular dynamics (MD) simulations. MD4 is a method to numerically solve the particle system problem. Currently, MD is used to simulate a variety of systems ranging from metals to large biomolecules. Our MD simulations were carried out using the “Lammps”5 code. The total energy of the system, $E$, for the closest “contact” between the molecule and the membrane provide a simple test to molecular permeability. If $E$ is positive, then we consider the sheet as impermeable to the molecule. In Table 1 we present these results for the different molecules considered here.

Table 1. Permeability test.

<table>
<thead>
<tr>
<th>Molecule</th>
<th>$E$ (x10^{-25} eV)</th>
<th>Permeability</th>
</tr>
</thead>
<tbody>
<tr>
<td>H₂</td>
<td>-147.04</td>
<td>+</td>
</tr>
<tr>
<td>He</td>
<td>-0.76</td>
<td>+</td>
</tr>
<tr>
<td>Ne</td>
<td>-1.12</td>
<td>+</td>
</tr>
<tr>
<td>O₂</td>
<td>12.08</td>
<td>-</td>
</tr>
<tr>
<td>Ar</td>
<td>17.08</td>
<td>-</td>
</tr>
<tr>
<td>CO₂</td>
<td>591.53</td>
<td>-</td>
</tr>
</tbody>
</table>

In Table 1, the energy $E$ is displayed in units of thermal energy at room temperature (300 K).

Conclusions
We have carried out MD simulations to test the BPC permeability to H₂, He, Ne, O₂, Ar and CO₂. Our results show that BPC membranes are permeable to hydrogen, helium and neon molecules, but impermeable to oxygen, argon and dioxide carbon molecules.

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References

Figure 1. The biphenylene carbon (BPC) structure.

Figure 2. The interaction between molecule and BPC.