# Selective permeability of graphenelyne membrane: performance in multifunctional gas separation

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## INTRODUCTION

Biphenylene carbon (BPC), also called graphenylene, is a hypothetical porous two-dimensional (planar) allotrope carbon[1] that may be obtained from selective dehydrogenation of porous graphene[2]. 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 to $H_2$, $CH_4$, $N_2$ and $CO_2$ gases. Also, we have evaluated the BPC selectivity for $CO_2/CH_4$, $CH_4$/N2, $CO_2/N_2$ and $H_2/CO_2$ gas mixtures.

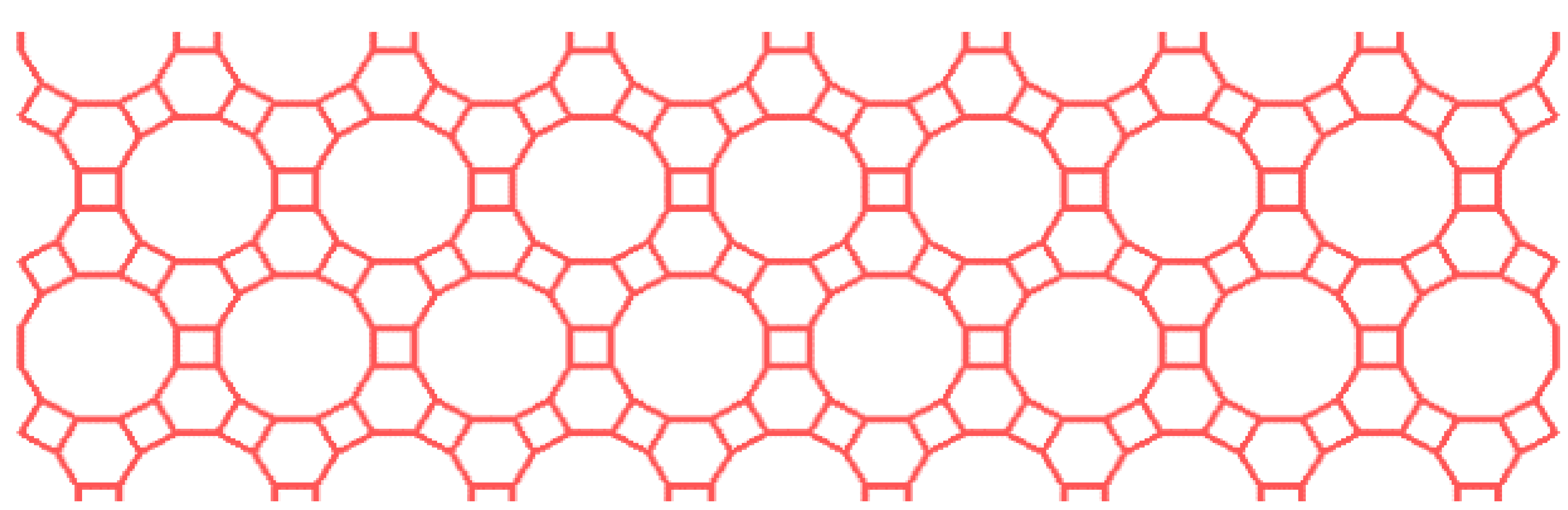

**Figure 1.** BPC is a porous carbon allotrope and has a thickness of a single atom. The BPC pores are regular decagons with a diameter of 3.2 Å.

## METHODOLOGY

In this work, fully atomistic MD simulations were performed to predict the gas adsorption and permeability of BPC to single $H_2$, $CH_4$, $N_2$ and $CO_2$ components. The simulation system consists of a single BPC sheet into contact with a gas reservoir under different pressure values (see Figure 2). The separation mechanism of the binary $CO_2/CH_4$, $CH_4$/N2, $CO_2/N_2$ and $H_2/CO_2$ gas mixtures was also evaluated.

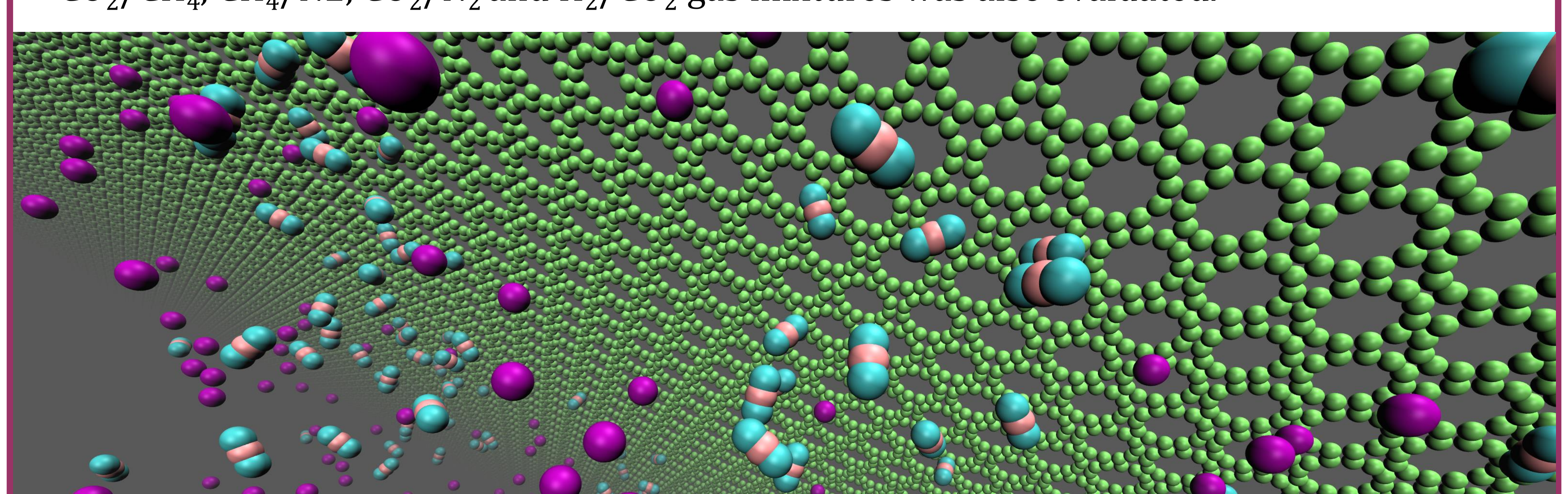

**Figure 2.** Simulation system.

## RESULTS AND DISCUSSION

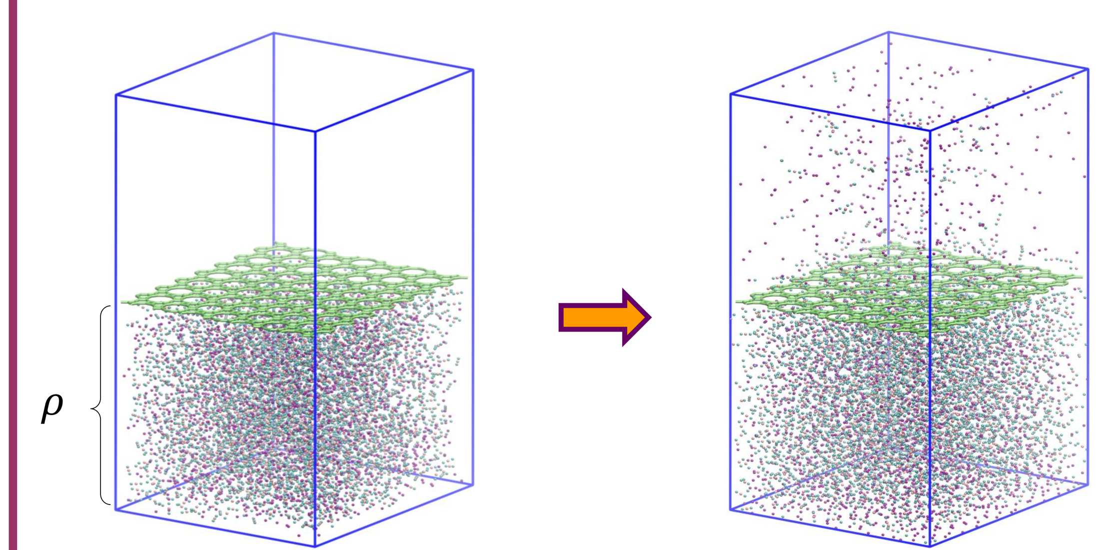


**Figure 3.** Snapshots of a $X/Y$ gas mixture system with a composition of 50% $X$:50% $Y$ in mols: on the **left**, the initial configuration at density $\rho$; on the **right**, the system in thermodynamic equilibrium at a temperature of 300 K.

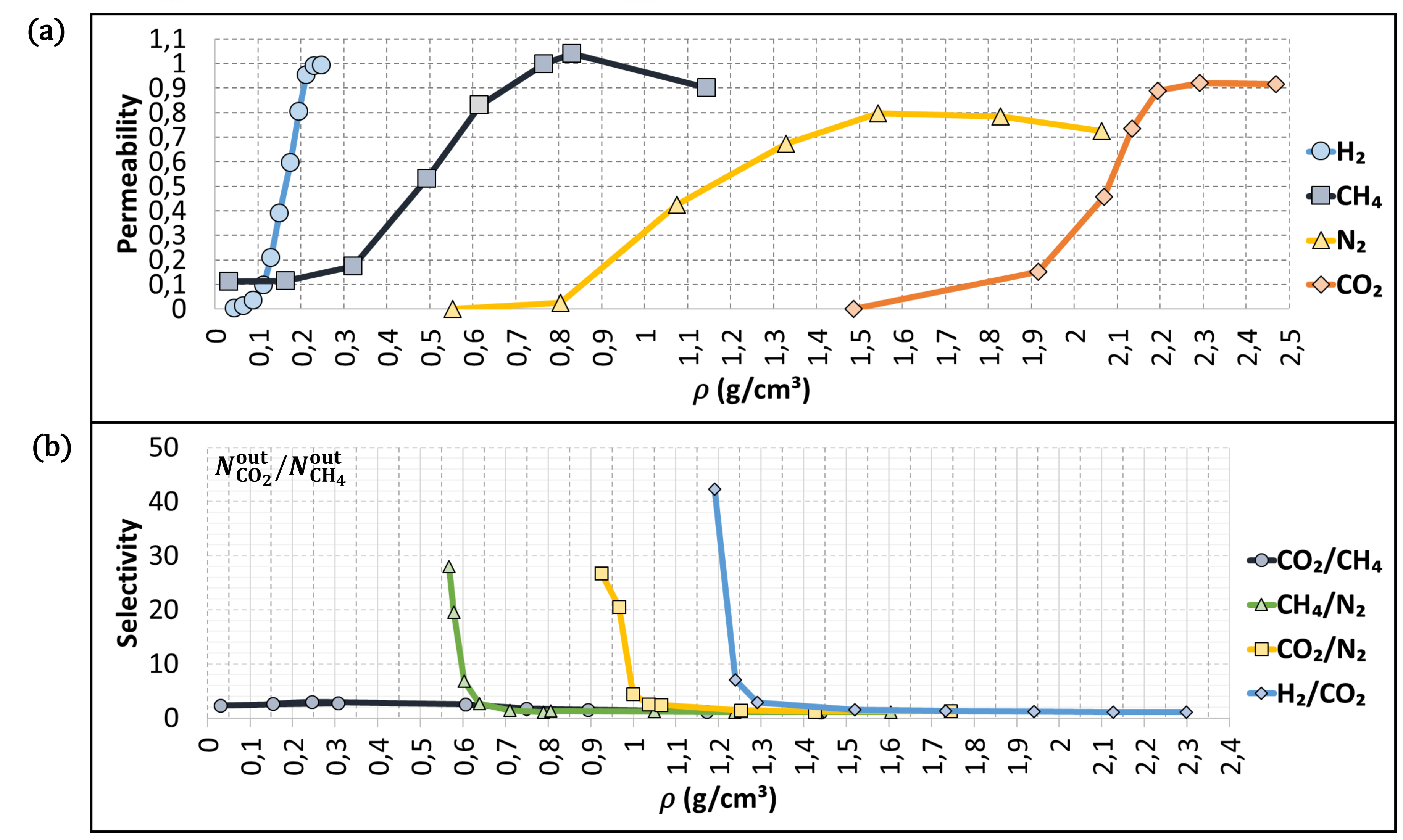


**Figure 4. (a)** BPC permeability (*i.e.* $P_X = N_X^{\text{out}}/N_X^{\text{in}}$) to $H_2$, $CO_2$, $CH_4$ and $N_2$ single components; **(b)** selectivity (*i.e.* $S_{X/Y} = N_X^{\text{out}}/N_Y^{\text{out}}$ ) at different initial densities and for each of the $CH_4$/N2, $CO_2/N_2$ and $H_2/CO_2$ mixtures. BPC exhibit high selective permeability for binary $CH_4$/N2, $CO_2/N_2$ and $H_2/CO_2$ gas mixtures depending on the reservoir pressure.

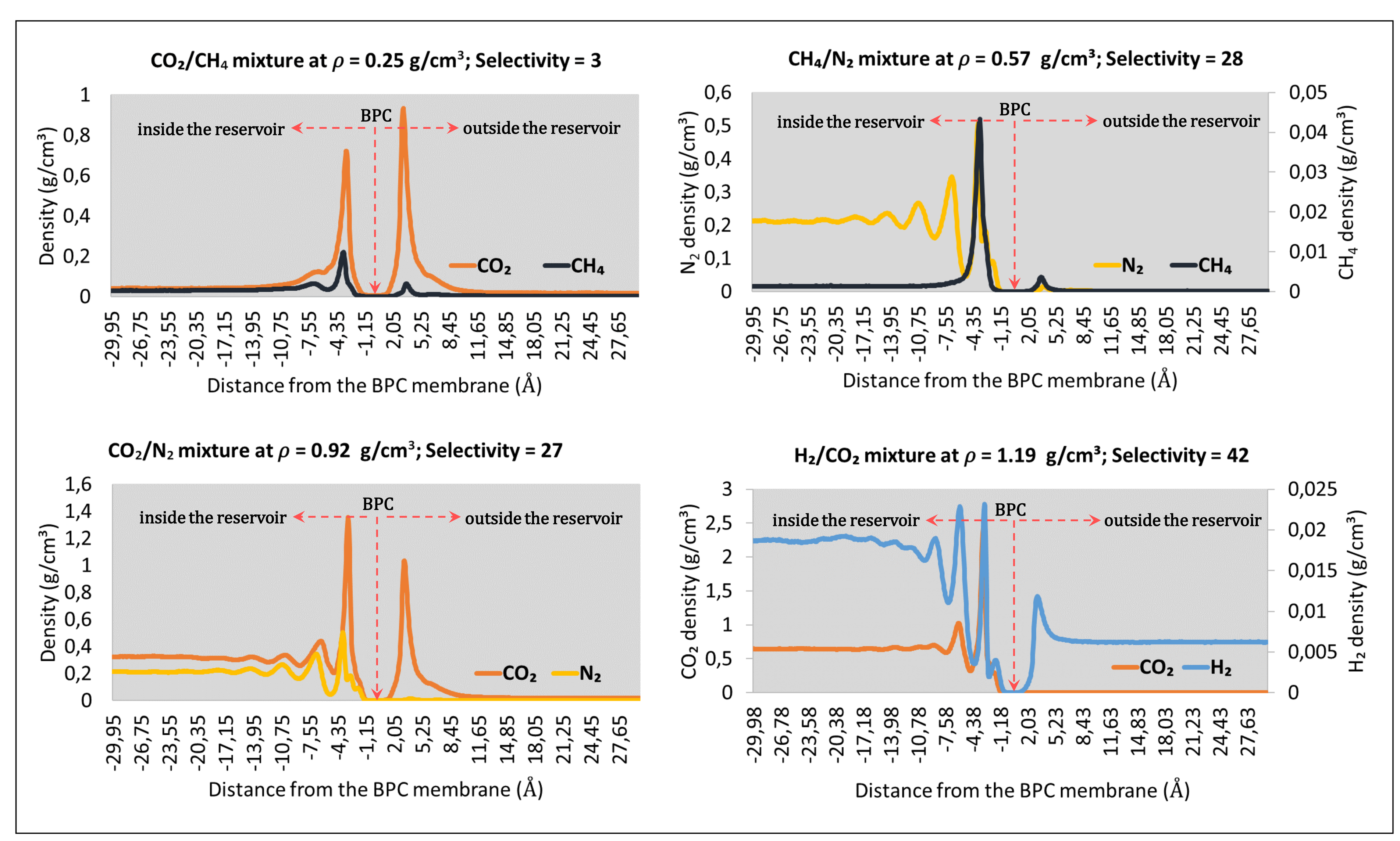


**Figure 5.** Density profile for each of the $CO_2/CH_4$ , $N_2/CH_4$, $CO_2/N_2$ and $H_2$/ $CO_2$ gas mixtures.

## CONCLUSIONS

Our results show that BPC is highly selective for $H_2$, $CO_2$ and $CH_4$, with good potential to work as a molecular sieve for the purification of these gases.

## REFERENCES

[1] K. S. Novoselov *et al.*, *Science* **306**, 666 (2004).
[2] J. S. Bunch *et al.*, *J. Phys. Cond. Mat.* **21**, 285304 (2009).
[3] R. H. Baughman, H. Eckhardt and M. Kertesz, *J. Chem. Phys.* **87**, 6687 (1987).
[4] Allen, M. P. and T. D. J. (1987). *Computer Simulations of Liquids.*
[5] Plimpton, S., *J. Comp. Phys.*, **117**, 1-19 (1995).

## ACKNOWLEDGMENTS

FAPESP
CNPq – Conselho Nacional de Desenvolvimento Científico e Tecnológico