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# Theoretical Study of Gas Diffusion through Porous Graphene under Pressure

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The gas separation properties of porous graphene (PG) membrane on $SiO_2$ substrate for simple molecules ($H_2$, $O_2$, and $CO_2$) under pressure have been investigated by using first-principles density functional theory. The van der Waals interaction was taken into account by using Grimme's force field (PBE-D2) approach [1]. For the clamped circular membrane subjected to a pressure difference between both sides of the membrane, the deformation of the membrane can be described by Hencky's solution [2]. The deformation of the membranes lowers the diffusion barriers for $H_2$, $O_2$ and $CO_2$ but by different amounts. This effectively increases the diffusion rate of $H_2$, $O_2$, and $CO_2$ by up to 4, 8, and 12 orders of magnitude, respectively (in the pressure range of 0-5 MPa). The selectivity or relative diffusion rate of PG for the diffusion of $H_2$, $O_2$, and $CO_2$ molecules at Deltap = 5 MPa relative to the $CO_2$ diffusion rate at Delta p = 0 MPa are 1024, 1019, and 1012, respectively. The results suggest that the gas separation properties of PG can be tuned by applying a pressure different across the membrane.

[1] S. Grimme, J. Comp. Chem. 27, 1787 (2006).
[2] W. B. Fichter, NASA Technical Paper, 3658 (1997).

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