# Water Flow Through Polar and Non-Polar Nanopores: Insights from Multiscale Simulation

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Abstract

In this study, we employ multiscale simulations to investigate the effect of water flow through nanopores in graphene and hexagonal boron nitride (hBN) membranes. Our results reveal a significantly higher water flow in hBN membranes than in graphene. This enhanced flow is attributed to the asymmetry of the hBN pores, which induces a dipole within the pore, as confirmed by quantum mechanics (QM) calculations. Classical molecular dynamics simulations further demonstrate that water molecules exhibit random distribution with no preferential orientation near the graphene pores, whereas a strong structuring is observed for hBN. Furthermore, hybrid quantum mechanics/molecular mechanics (QM/MM) simulations indicate that the dipole moment of the hBN pore increases in the presence of water, as evidenced by the average charge distribution. Conversely, the symmetric nature of graphene pores results in non-polar characteristics, as verified by both QM/MM and QM calculations. These findings provide valuable insights into the distinct water transport properties when flowing through graphene and hBN nanopores, with potential implications for the design of advanced nanofiltration membranes [1-3].

References

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[3] Mendonça, B. H., de Moraes, E. E., Batista, R. J., de Oliveira, A. B., Barbosa, M. C., Chacham, H. (2023). The Journal of Physical Chemistry C, 127(20), 9769-9778.

Figures

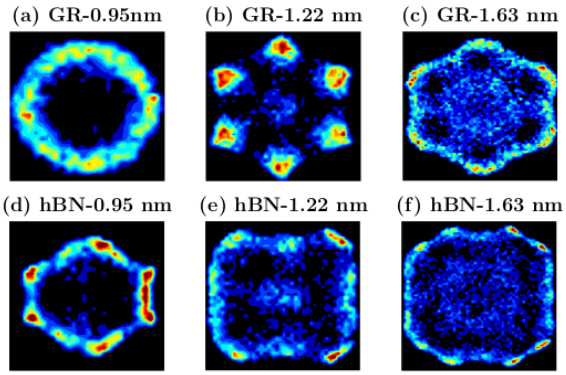


**Figure 1:** Oxygen density maps for P = 100MPa