Exploring optimal graphene slit-pore width for the physical separation of water-methanol mixture.

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Efficient and sustainable techniques for separating water- alcohol mixtures are in high demand in the industry. Recent research has revealed that nanotechnology could be the optimal solution. In this study, we investigate how the width of a nano-confining graphene slit-pore affects the filtration and purification of water-methanol mixtures. Using Molecular Dynamics simulations of a coarse-grained model for mixtures containing up to 25 percent methanol, we found that specific pore sizes segregate the two components, with water being preferred in the centre and methanol accumulating near the hydrophobic walls. Altering the pore width also affects non-monotonically the diffusivity of each component, with water diffusing faster than methanol. Hence, optimal pore size, leveraging segregation and diffusion differences, can enable the successful extraction of both components. However, the system requires external forces and work to maintain mechanical stability at specific pore widths. Our research indicates that 12.5 Å pore size maximizes physical separation, ensuring that the energy cost of a filtering graphene membrane is minimized.

References

[1] R. Bellido-Peralta, F. Leoni, C. Calero, and G. Franzese, Journal of Molecular Liquids, vol. 391, p. 123356, 2023
[2] F. Leoni, C. Calero, and G. Franzese ACS Nano, vol. 15, no. 12, pp. 19864–19876, 2021.
[3] M. S. Marques, V. F. Hernandes, E. Lomba, and J. Bordin, Journal of Molecular Liquids, vol. 320, p. 114420, 2020
[4] M. Huš and T. Urbic, Physical Review E, vol. 90, no. 6, p. 062306, 2014.

Figures

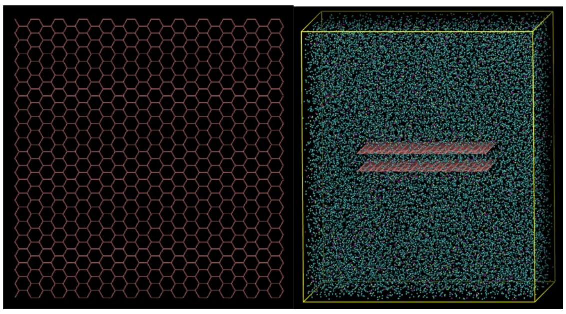

Figure 1: Visualization of the simulated system. Detail of the designed graphene walls (left) and an overall sight of the whole system with the slit-pore in the centre (right).