Gas permeation through graphdiyne-based nanoporous membranes

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Abstract

Two dimensional membranes having angstrom-scale pores are under extensive research investigation due to its promising capabilities of exponential selectivity with high permeation rates. Recent report[1] on monolayer graphene with single pore limit shows exponential selectivity. Although it shows the performance beyond Robeson bound for polymers (100nm thickness), the flow rates are not as high as required for the technological requirements. Therefore, we investigate[2] graphdiyne membrane (90nm thickness) with intrinsic pores, using isotopes and cryogenic temperature, to explore beyond the selectivity-permeability trade-off limits. Despite being nearly a hundred of nanometers thick, the membranes allow fast, Knudsen-type permeation of light gases such as helium and hydrogen whereas heavy noble gases like xenon exhibit strongly suppressed flows. Beyond steric exclusion, there are other factors including lattice flexibility and adsorption that affect selectivity between gases. Furthermore, the unexpected fast permeation combined with selective gas transport through graphdiyne provide a better permeability-selectivity trade-off compare to that of state-of-art membranes, beyond the existing bounds. Our work offers important insights into intricate transport mechanisms playing a role at nanoscale. Our study provides a feedback on the extensive theoretical[3] simulations of molecule sieving through graphdiyne with intrinsic lattice pores in angstrom scale.

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