Abstract Submitted
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Molecular Dynamics Simulation of Gas Separation using Nanoporous Graphene[1] HAROLD AU, MICHAEL BOUTILIER, Mechanical Engineering Dept., MIT, PIETRO POESIO, Dept. of Mechanical and Industrial Engineering, Brescia University, Italy, NICOLAS HADJICONSTANTINOU, ROHIT KARNIK, Mechanical Engineering Dept., MIT — We present molecular dynamics simulations of gas transport through nanoporous graphene to evaluate the latter's potential as a gas-separation membrane. Due to their very small thickness, such membranes are expected to exhibit high permeance. Provided precise tuning of the pore sizes is possible, graphene membranes have the potential to combine high permeance with high selectivity through molecular size exclusion. In the present study, we focus on separation of methane from hydrogen. Our results show that graphene with pores that are large compared to the kinetic diameters of both species are permeable to both gases. As pore size is reduced, we observe a greater decrease in the permeance of methane that results in a size exclusion effect for a range of pore sizes that are still permeable to hydrogen. Our results indicate that hydrogen permeance over this range of pores sizes is sufficiently large to offer considerable improvement compared to state of the art polymeric membranes.

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