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Molecule permeation and gas separation by nanoporous graphene membranes[1] NICOLAS HADJICONSTANTINOU, CHENGZHEN SUN[2], MICHAEL BOUTILIER, ROHIT KARNIK, MIT — Molecular simulations and experiments suggest that by introducing nanopores of appropriate size, nanoporous graphene membranes can exhibit permeability and selectivity exceeding those of existing state-of-the-art membranes by several orders of magnitude. To better understand how gases permeate through these membranes, we conducted molecular dynamics simulations of gas permeation through different nanopores for four different gases, namely helium, hydrogen, nitrogen and methane. Our results show that in addition to the direct flux, defined as the contribution from molecules crossing directly from the gas-phase on one side of the graphene to the other, in some gases, significant contribution to the flux across the membrane comes from a surface mechanism, in which the molecules cross after being adsorbed onto the graphene surface. Our results quantify the relative contribution of the bulk and surface mechanisms and show that the direct flux can be described reasonably accurately using kinetic gas theory, provided the latter is appropriately modified to account for finite-molecule-size effects by assuming steric interactions between rigid pores and hard-sphere gas molecules of known kinetic diameters.

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