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Highly selective sieving in porous graphene-like carbon nitride for helium/light isotopes separation

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An efficient membrane for helium separation from natural gas is quite crucial for cryogenic industries. However, most experimentally available membranes fail in separating helium from small molecules in natural gas, such as H_2, as well as in $^3He/^4He$ isotopes separation. Using first-principles calculations, we theoretically demonstrated that the already-synthesized graphitic carbon nitride (g-C_3N_4) has high efficiency in helium separation from the gas molecules (H_2, N_2, CO and CH_4) in natural gas and the noble gas molecules (Ne and Ar). The selectivity of He over H_2 molecule at room temperature is calculated to be as high as 10^7. More interestingly, the g-C_3N_4 membrane can also serve as a quantum sieving membrane for $^3He/^4He$ separation with a predicted transmission ratio of 18 at 49 K, thus offers a combined means of both He and ^3He isotope separation. Furthermore, for another experimentally available porous graphene-like carbon nitride (C_2N-*h*2D), we theoretically demonstrated that highly efficient light isotopes separation, such as $^3He/^4He$, can be reached via quantum sieving effect. Under moderate tensile strain, the quantum sieving of the C_2N-*h*2D membrane can be effectively tuned in a continuous way, leading to a temperature window with high $^3He/^4He$ selectivity and permeance acceptable for efficient isotopes harvest in industrial application. This mechanism also holds for separation of other light isotopes, such as H_2/D_2, H_2/T_2. Such tunable quantum sieving opens a promising avenue for light isotopes separation for industrial application.

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