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## Mechanistic insights into porous graphene membranes for helium separation and hydrogen purification

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### Abstract

Porous graphene (PG) and nitrogen-substituted PG monolayers of 3N-PG and 6N-PG were designed as effective membranes for the separation of He and H<sub>2</sub> over Ne, Ar, N<sub>2</sub>, CO, and CH<sub>4</sub> by using density functional theory. Results showed that PG and 3N-PG exhibited suitable pore sizes and relatively high stabilities for He and H<sub>2</sub> separation. PG and 3N-PG membranes also presented excellent He and H<sub>2</sub> selectivities over Ne, Ar, N<sub>2</sub>, CO and CH<sub>4</sub> at a wide temperature range. 6N-PG membrane exerted unexceptionable permeances of the studied gases, especially He and H<sub>2</sub>, which could remarkably improve the separation efficiency of He and H<sub>2</sub>. Analyses on the most stable adsorption configurations and maximum adsorption energies indicated weak Van der Waals interactions between the gases and the three PG-based membranes. Microscopic permeation process analyses based on the

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