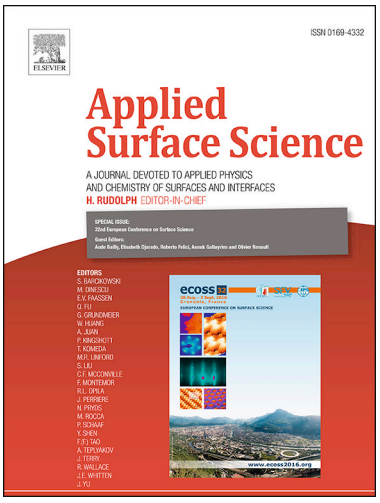

Full Length Article

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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_2 over Ne, Ar, N_2, CO, and CH_4 by using density functional theory. Results showed that PG and 3N-PG exhibited suitable pore sizes and relatively high stabilities for He and H_2 separation. PG and 3N-PG membranes also presented excellent He and H_2 selectivities over Ne, Ar, N_2, CO and CH_4 at a wide temperature range. 6N-PG membrane exerted unexceptionable permeances of the studied gases, especially He and H_2, which could remarkably improve the separation efficiency of He and H_2. 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