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Nanoscale Study of CO2/CH4 Separation through Two-stage Nanoporous Graphene Membranes[1] NAIYER RAZMARA, Department of Mechanical Engineering, Escola Politcnica, University of So Paulo, So Paulo, SP, Brazil, ALEXSANDRO KIRCH, DANIELA ANDRADE DAMASCENO, Instituto de Fsica, Universidade de So Paulo, CP 66318, So Paulo, SP 05315-970, Brazil, JULIO ROMANO MENEGHINI, Department of Mechanical Engineering, Escola Politcnica, University of So Paulo, So Paulo, SP, Brazil, CAETANO RODRIGUES MIRANDA, Instituto de Fsica, Universidade de So Paulo, CP 66318, So Paulo, SP 05315-970, Brazil — During the last decade, various designs have been introduced to separate CH_4 from other components in gas mixtures. The development of effective membranes with high selectivity and permeability is one of the most challenging subjects in carbon capturing and storage. In this context, we investigated the transport and separation of CO_2/CH_4 binary mixture through a two-stage bilayer nanoporous graphene design. The molecular dynamics technique is applied to investigate the transport properties. Benchmarked forcefields are adopted for modeling the interactions between different molecules. Three boxes are considered as feeding, transferring, and capturing reservoirs. Three configurations of nanoporous graphene membranes are examined, namely, in-line, offset of 10 angstroms, and offset of 20 angstroms. The simulation results indicate that increasing the offset distance leads to a considerable decrease in the number of CH_4 molecules in the CO_2 capturing reservoir. This study suggests one of the practical designs for the separation of CH_4 with the application in the CO_2 abatement industry.

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