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CO_2 separation using a porous graphene/IL membrane JOONHO LEE, NARAYANA R. ALURU, Department of Mechanical Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, IL 61801 — We investigated the separation of CO_2 from CO_2/O_2 mixture using a porous graphene/ionic liquid (IL) membrane. By performing extensive non-equilibrium molecular dynamics (NEMD) simulations, we observed dramatic CO_2 separation with a 0.99 nm graphene nanopore. By calculating the density distribution, we show that a strong layering of the ionic liquid is observed near the 0.99 nm graphene nanopore, while such a strong layering is not observed in the larger 2.22 nm diameter pore. The strong layering induces a near perfect blockage of O_2 molecules from diffusing into the ionic liquid. Void analysis shows that the layering of ionic liquid serving as a blockage for O_2 molecules does not hinder CO_2 solvation in the ionic liquid.

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