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Ionic-Functionalized Polymeric Microporous Materials SHALINI J. RUKMANI, Department of Materials Science and Engineering, University of Florida, THILANGA LIYANA-ARACHCHI, Department of Chemistry, University of Florida, KYLE HART, Department of Materials Science and Engineering, The Pennsylvania State University, CORAY COLINA, Department of Chemistry, University of Florida — Ionic-functionalized microporous materials are attractive for gas adsorption and separation applications. In this study, we investigate the effect of changing ions (Li^+, Na^+, K^+, Rb^+, and Mg^{2+}) on the porosity, carbon dioxide (CO_2) gas adsorption, and selectivity in ionic functionalized polymers of intrinsic microporosity (IonomIMs). Structure generation and gas adsorption are studied using molecular dynamics and Monte Carlo simulations respectively. The IonomIMs show an enhanced performance for CO_2 selectivity in CO_2/CH_4 and CO_2/N_2 gas mixtures at pressure swing adsorption and vacuum swing adsorption conditions. For 100% ionic concentration, ions with the same charge show a decrease in the adsorption capacity with increasing cation size. Mg^{2+} has the highest pure CO_2 adsorption and lowest mixed gas separation performance. The increasing concentration of ions decreases the porosity of the framework and increases the tunability of structural and adsorption properties. Hence, the concentration of ions, size, and charge play a vital role in determining the optimum adsorbent for a targeted industrial application.

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