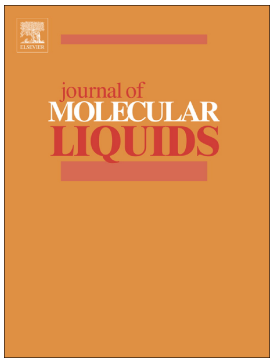

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Molecular-level understanding of supported ionic liquid membranes for gas separation

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Abstract

Supported Ionic Liquid Membranes (SILMs) have found wide applications in gas separation and purification, especially for CO_2 capture. In this study, a molecular level approach was investigated in order to analyze various types of ILs for use in SILMs and consequently evaluation of membranes performance using quantum molecular chemical modeling and calculations. Relationships were developed for the permeability and selectivity of SILMs and then validated using collected experimental data of relevant gas pairs in separation applications. To calculate the concentration of gas in various ILs and diffusivity calculations, a COSMO-based activity coefficient model and the mean square displacement determined using some quantum mechanics simulations were used respectively, and were then validated using collected experimental data to ensure consistency of model. In order to compare and evaluate the model performance, the accumulative absolute relative deviation (AARD (%)) was used. The presented approach gives accurate, pure predictive, extendable and reproducible method