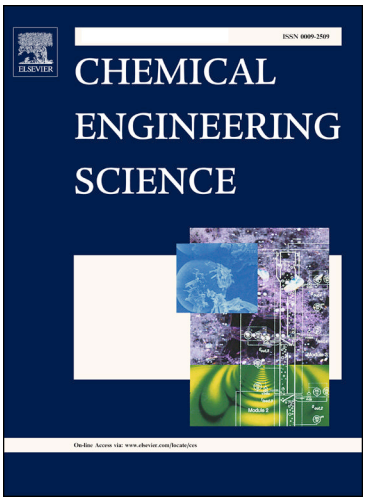

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Gas separation by ionic liquids: A theoretical study

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Abstract

Ionic liquids (ILs) have great potential for separating gases as well as avoiding solvent loss and environmental pollution. An in-depth understanding of the interaction mechanism between ILs and gases is extremely important for exploring and developing high-performing ILs for gas separation. Quantum chemistry is a powerful approach for gaining insight into separation mechanisms. Herein, with the aid of this method, the interaction mechanisms of three representative ILs, i.e., diethylmethylsulfonium tricyanomethane ($[S_{221}][CCN_3]$),

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