

Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Carbon dioxide and methane transport in DDR zeolite: insights from molecular simulations into carbon dioxide separations in small pore zeolites SANG EUN JEE, DAVID SHOLL, Georgia Institute of Technology, EXXON MOBIL CORPORATION COLLABORATION — Zeolites are good candidates as a membranes for chemical separations because of their excellent chemical and thermal stability. Cage type zeolites are promising materials for gas separation since their narrow windows are expected to control molecular transport. DDR is one of the strongest candidates for light gas separations because of its narrow 8MR window. In our study, we examined the separation selectivity of DDR for CO₂/CH₄ separation using atomistic simulation methods. We introduced new force fields which can reproduce experimental single component adsorption and diffusion data for this material for the first time. Previously interatomic potentials that have been applied to DDR overestimate experimental diffusivities at least one order of magnitude. We characterized single-component and binary adsorption using Grand Canonical Monte Carlo, and single-component diffusion using a combination of Molecular Dynamics and Transition State Theory. The most important observation from our calculation is that CO₂/CH₄ diffusion in DDR is very different from the usual situation in nanoporous materials, where the presence of a slowly diffusing species retards transport rates of a more rapidly diffusing species. In DDR, we show that CO₂ diffusion rates are only weakly affected by the presence of CH₄, despite the very slow diffusion of the latter species. The physical origins of this unusual behavior are explained by analyzing the adsorption sites and diffusion mechanism for each species.

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Date submitted: 08 Jan 2009

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