

**Separation of Ethanol and Water using Solvents or Zeolites:
Molecular-level Insights from Simulation Studies**

J. Ilja Siepmann^{C,S}, Peng Bai and Samuel L. Keasler

*University of Minnesota, Depts. of Chemistry and of Chem. Eng. and Mats. Sci., Minneapolis, MN, U.S.A.
siepmann@umn.edu*

Configurational-bias Monte Carlo simulations in the Gibbs ensemble and the TraPPE force field are used to explore liquid-liquid extraction and zeolite-based sorption processes for the separation of ethanol and water. Effects of temperature and feedstock composition are investigated. The simulations provide molecular-level insights on how the architecture of primary, secondary, and tertiary long-chain alcohols and of hydrophobic zeolites influence separation selectivity and capacity.