Monte Carlo Simulations for Water/N-Alkane/1-Alkanol Mixtures

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Multi-component mixtures that exhibit a liquid-liquid miscibility gap are of utmost importance for the oil and gas industries because of the prevalence of hydrocarbons and water in many processes. Here we present configurational-bias Monte Carlo simulations in the Gibbs ensemble to investigate the phase behavior and structure of ternary water/(n-hexane or n-dodecane)/(ethanol or 1-propanol) mixtures. Analysis of the simulation trajectories yields a wealth of information on microheterogeneous features of the liquid phases.