Molecular Dynamics Simulations for Phase Transitions of Water/Poly(ethylene oxide) (PEO) Solutions

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A lower critical solution temperature (LCST) behaviors of water/poly(ethylene oxide) (PEO) solutions were examined by means of molecular dynamics (MD) simulations. A careful MD procedure is established based on the corresponding experiments so that the correct surrounding conditions of the simulated cells are constructed. We computed radial distribution functions, number of hydrogen bonds, energy of mixing, mean-squared displacements, and radius of gyration with respect to the temperature. We found that hydrogen bonds between PEO and water decrease more rapidly than those of water and water with increasing temperature, indicating lower critical solution temperature (LCST) behavior. In the heterogeneous phase temperature range, both mixing energy and radius of gyration showed lower values than those of the homogenous phase, which corresponds well with the LCST type miscibility behavior.