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Conformations and Structure in Aqueous Poly(ethylene oxide) Solutions

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Atomistic molecular dynamics (MD) simulations have resulted in important insights into the influence of water on the local conformations and chain dimensions of poly(ethylene oxide) (PEO) as well as the role of PEO-water polar interactions and PEO-water and water-water hydrogen bonding interactions on solution structure as a function of composition and temperature. Results of these simulations will be presented and discussed. In addition, results of recent simulation studies of PEO brushes and the interaction of PEO-modified nanoparticles in aqueous solution will be considered.