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Molecular dynamics simulations of coil-helix transition of polyethylene oxide in solution and in presence of carbon nanotube. UDAYA DAHAL, ELENA DORMIDONTOVA, University of Connecticut — Hydrogen bonding between polymer and solvent determines macromolecular properties, e.g. conformation, in solution as well as under nanoconfinement. Using atomistic molecular dynamics simulations, we investigate the dynamics and conformation of polyethylene oxide (PEO) in water, isobutyric acid and in presence of a carbon nanotube (CNT). We found that, isobutyric acid hydrogen bonded to PEO has longer residence lifetime than hydrogen bonded water in aqueous solution. We show that this higher stability of hydrogen bonded solvent is responsible for helix-like PEO conformation in isobutyric acid solution compared to coil-like conformation of PEO in aqueous solution. Under the presence of a CNT, we find that PEO spontaneously enters the CNT from aqueous solution and forms rod-like, helix and wrapped chain conformation depending on CNT diameter. The helix formation under nanoconfinement is attributed to the stable water arrangement around PEO inside the CNT. We further discuss the implication of hydrogen bond stability and solvent arrangement for PEO chain conformation and mobility.

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