Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Molecular dynamics simulations of poly (ethylene oxide) hydration and conformation in solutions.[1] UDAYA DAHAL, DDept. of Physics and Inst. of Mat. Sci., Univ of Connecticut, ELENA DORMIDONTOVA, Dept. of Physics and Inst. of Mat. Sci., Univ of Connecticut — Polyethylene oxide (PEO) is one of the most actively used polymers, especially in biomedical applications due to its high hydrophilicity, biocompatibility and potency to inhibit protein adsorption. PEO solubility and conformation in water depends on its capability to form hydrogen bonds. Using atomistic molecular dynamics simulations we investigated the details of water packing around PEO chain and characterized the type and lifetime of hydrogen bonds in aqueous and mixed solvent solutions. The observed polymer chain conformation varies from an extended coil in pure water to collapsed globule in hexane and a helical-like conformation in pure isobutyric acid or isobutyric acid –water mixture in agreement with experimental observations. We'll discuss the implications of protic solvent arrangement and stability of hydrogen bonds on PEO chain conformation and mobility.

[1]This research is supported by NSF (DMR-1410928)

Udaya Dahal
Dept. of Physics and Inst. of Mat. Sci., Univ of Connecticut

Date submitted: 24 Nov 2015 Electronic form version 1.4