

Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Structure and flow properties of micelle-nanoparticle solutions from Molecular Dynamics simulations¹ RADHAKRISHNA SURESHKUMAR, SUBAS DHAKAL, ABHINANDEN SAMBASIVAM, Department of Biomedical and Chemical Engineering, Syracuse University, Syracuse, NY 13244 — In aqueous media, cationic surfactant molecules spontaneously self-assemble into diverse morphologies depending upon temperature, surfactant concentration and solution ionic strength. Spherical, cylindrical and long (\sim microns) flexible wormlike structures with or without branches with distinct rheological properties are observed. Inclusion of nanoparticles (NPs) provides additional means to manipulate structure and create active “nano-fluids” that respond to optical, magnetic or electrical stimuli. We study self-assembly, dynamics and rheology of such fluids using coarse-grained Molecular Dynamics simulations in presence of explicit solvent and salt. Specifically, we will discuss the mechanisms underlying fascinating phenomenology observed experimentally such as the pronounced non-monotonic dependence of the zero shear viscosity on salt/NP concentration, shear-induced structure formation, and isotropic to nematic transitions.

¹NSF grants 1049489, 1049454 for the financial support, and Pittsburg Super Computer Centre for providing HPC resources.

Subas Dhakal
Department of Biomedical and Chemical Engineering,
Syracuse University, Syracuse, NY 13244

Date submitted: 14 Nov 2013

Electronic form version 1.4