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Topology, Energetics and Rheology of Surfactant Micelles¹ RAD-HAKRISHNA SURESHKUMAR, SUBAS DHAKAL, ABHINANDAN SAMBASI-VAM, Syracuse University — A rich variety of self-assembled structures of amphiphilic molecules, ranging from spherical and cylindrical shapes to topologically complex networks consisting of branches and loops, is unraveled through large scale Molecular Dynamic simulations that account for explicit solvent, electrostatic and hydrodynamic interactions. The simulations employ a coarse grained force field, benchmarked against atomistic simulations (Sangwai and Sureshkumar, Langmuir, 27, 6628 (2011); 28, 1127 (2012)), to describe inter-molecular forces. Analysis of these structures allows for the first time to directly determine certain fundamental length scales, e.g. persistence and contour lengths, mesh size, as well as the end cap energy, which dictate the rheological properties and flow phenomena in micellar fluids. The much debated anomalous viscosity variations with respect to salt concentration can be understood based on the underlying morphological changes (http://arxiv.org/abs/1407.5086). This, and the effect of nanoparticle addition to the network structure and flow properties, will be discussed.

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