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Molecular Dynamics simulations of flow-structure interactions in fluids containing cylindrical micelles and micelle-nanoparticle complexes[1]
RADHAKRISHNA SURESHKUMAR, Syracuse University, Syracuse, NY, ASHISH SANGWAI, Intel Corporation, Hillboro, OR, ABHINANDEN SAMBASIVAM, Syracuse University, Syracuse, NY, SYRACUSE UNIVERSITY TEAM — Coarse-grained (CG) force fields, benchmarked against fully atomistic ones, are used in Molecular Dynamics simulations to predict shape transitions and binary interactions in cationic surfactant micelles as well as to understand the molecular mechanisms of self-assembly of micelles with noble metal nanoparticles germane to plasmonics. Non-equilibrium MD simulations are conducted to probe the effect of flow shear on cylindrical micelle dynamics and estimate properties such as tumbling frequency, relaxation time and scission energy. Simulations are also performed to understand flow-mediated alignment and merger of two cylindrical micelles which is hypothesized to be the mechanism underlying the formation of shear-induced structures in micellar fluids.

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Radhakrishna Sureshkumar
Syracuse University, Syracuse, NY

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