Modeling Stimuli-Responsive Nanoparticle Monolayer XIN
YONG, State Univ of NY - Binghamton — Using dissipative particle dynamics
(DPD), we model a monolayer formed at the water-oil interface, which comprises
stimuli-responsive nanoparticles. The solid core of the nanoparticle encompasses
beads arranged in an fcc lattice structure and its surface is uniformly grafted with
stimuli-responsive polymer chains. The surface-active nanoparticles adsorb to the
interface from the suspension to minimize total energy of the system and create a
monolayer covering the interface. We investigate the monolayer formation by char-
acterizing the detailed adsorption kinetics. We explore the microstructure of the
monolayer at different surface coverage, including the particle crowding and order-
ing, and elucidate the response of monolayer to external stimuli. The collective
behavior of the particles within the monolayer is demonstrated quantitatively by
vector-vector autocorrelation functions. This study provides a fundamental under-
standing of the interfacial behavior of stimuli-responsive nanoparticles.

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