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 characterizing the detailed adsorption kinetics. We explore the microstructure of the monolayer at different surface coverage, including the particle crowding and ordering, 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 understanding of the interfacial behavior of stimuli-responsive nanoparticles.