Abstract Submitted
for the SES14 Meeting of
The American Physical Society

Physical principle for the pattern formation of binary self-assembled monolayer on nanoparticle surface XINWEI GE, FENG DING, Clemson Univ, DING RESEARCH LAB TEAM — Self-assembled monolayer (SAM) where ligand molecules spontaneously assemble on nanoparticle (NP) surface is a common approach to stabilize or functionalize NPs. It has been proposed that a binary SAM of mixing two immiscible ligands can form stripe-like patterns on NP surfaces, which may induce novel functions. Experimental characterizations and computational simulations had been performed to show this conformation could form spontaneously on gold NPs. However, previous evidences were questioned due to their limitations. The principle for pattern formation is still not conclusive yet. We applied atomistic discrete molecular dynamics (DMD) simulation to study the binary SAM on gold NPs and our results showed that pattern conformation can indeed form on NPs surface only if favorable conditions are satisfied. The formation of patterns depends on physicochemical characteristics of composite ligands and thus relative interactions between them. Temperature also plays a role here as patterns eventually disappear at high temperature where random distribution with high entropy is favorable. We proposed a simple thermodynamics-based theory that can estimate pattern formation in a binary SAM and also demonstrate the application of this principle.

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Date submitted: 03 Oct 2014 Electronic form version 1.4