Title: Computational Design of Coatings/Functionalization on Particle Surfaces for Particle Stabilization in Formulations and Suspensions
PI: Arthi Jayaraman (University of Delaware)
Number of Graduate Students/Post Docs: 1 Postdoc
Time span: Two years
Budget: $200,000/2yr (this is with no overhead)

Abstract: In this project PI Jayaraman will develop and use state-of-the-art molecular simulations and theory to understand how the functionalization/coating on organic/inorganic nanoparticles alters the state of particle dispersion within industrially relevant formulations or suspensions (e.g., lotions, inks, paints, etc.). The coating design ranging from polymers to oligomers as well as surfactants will be linked to observed microstructure and dynamics within industrial relevant solutions.

Summary of Project: Many of the products of interest to industrial partners of the CHEM IUCRC (e.g., paints, inks, formulations for personal care and cosmetics) are made of solutions containing nanoscale additives (particles). Understanding ways to stabilize the dispersion of nanoparticles within these solutions or dense suspensions is vital for improving the user applicability, shelf-life and efficacy of these products. PI Jayaraman will use computational tools like liquid state theory and molecular simulations [1,2] to explore a vast number of material parameters and conditions to identify the optimal molecular design rules that accomplish this goal of improved particle dispersion and explain the underlying mechanisms that lead to such behavior.

Aims of the Project: In the proposed project, Jayaraman and her team will leverage their extensive past expertise with atomistic and coarse-grained simulations and theory studies of polymer-particle solutions and composites (**Figure 1**) [e.g. Refs. 3-10] to

1. study a broad range of feasible (based on cost, chemistry and synthesis as stipulated by the industry) surface functionalization on the nanoparticle at industrially relevant conditions (temperature, pressure, composition),
2. quantify structure (particle dispersion or assembly, relative arrangement of other additives and nanoparticles) and thermodynamics (e.g.,

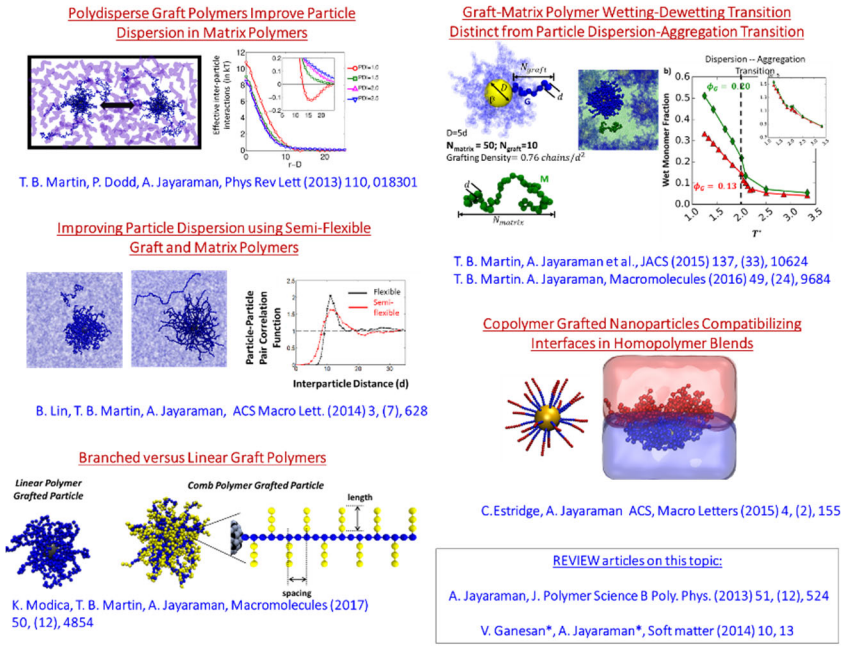

Figure 1. *Some of the past work from PI Arthi Jayaraman's research group on particle-polymer systems.*

effective interactions, second virial coefficients, phase behavior with changing temperature) and as a function of the materials design parameters and conditions.

As she has been doing in many of her other experimental-computational collaborations [e.g., Refs. 12-18], Jayaraman will harness the powerful feedback loop between the computational work in her lab and ongoing experiments within the industrial labs and other research groups within NSF CHEM IUCRC to validate the models and simulation methods. She will then use the validated model and method to make predictions that guide ongoing and new experimental work in the labs of the industrial partner(s).

Outcome of the Project: The project will result in a library of computationally derived materials design rules for coatings/functionalization that lead to stable particle dispersions in formulations/solutions/slurries of relevance to the industrial partner.

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