RX17-6

Structure-Property Correlations of Polymer-Grafted Nanoparticles on Surfaces

1. **Research Title:** Structure-Property Correlations of Polymer-Grafted Nanoparticles on Surfaces
2. **Individual Sponsor:**

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3. **Academic Area/Field and Education Level:** Materials Science and Engineering, Chemical Engineering, Chemistry, or Physics (MS or PhD level)

4. **Objectives:** Through theory and/or coarse grain simulations, develop a macromolecular-level understanding of the behavior of polymer-grafted nanoparticles (or hairy nanoparticles, HNPs) on surfaces. Of special interest are predictions of how the architecture of the HNP and the surface relates to (1) the height profile of the polymer canopy around a single adsorbed HNP, (2) the relaxation modes of the polymer canopy, and (3) the number of polymer entanglements within the canopy, with a polymer brush surface, and between canopies of two or more nearby adsorbed HNPs. The first will allow validation of theory and/or coarse grain simulations versus existing experimental results, while the latter two are important consideration underlying the plasticity and toughness of these systems.

5. **Description:** Polymer-grafted nanoparticle systems are a class of inorganic-organic hybrid materials in which the volume fraction and spacing of the inorganic constituents can be precisely tuned by adjusting polymer length and grafting density. HNPs can be deposited on surfaces at various controlled densities, making them promising for specialty printing applications or to create an array of hexagonally packed particles with attractive mechanical and optical properties. However, while a large body of prior work is available to describe how HNPs can be used as additives to adjust the properties of polymer melts, much less is known about how to control their behavior on surfaces.

   This effort will use theory and/or coarse grain simulations to reveal the polymer conformations, entanglement network, and local dynamics that determine HNP behavior on surfaces. Also of interest is a prediction of how solvent swelling and a densely grafted polymer brush on the substrate alter the HNP absorption behavior. These fundamental insights will be considered in context to what is known of linear chains, dendrimers and block-copolymers on surfaces; and thereby develop a broader understanding of how molecular-scale architecture impacts the behavior of ultra-thin macromolecular films. These insights will guide future experimental work in crafting well ordered, reproducible, and mechanically robust arrays of particles for use in specialty printing, optical devices, or other applications.
6. **Research Classification/Restrictions:** Unrestricted
7. **Eligible Research Institutions:** Indicate to what organizations this topic should be provided

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