RX18-13

1. **Research Title:** Molecular Design of Polymer-Grafted Nanoparticles for Next Generation Printed Electronics and Energy Storage

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 grained simulations, develop a macromolecular-level understanding of the behavior of polymer-grafted nanoparticles (PGN) on surfaces. Of special interest are predictions of how the molecular-level architecture of the PGN relates to (1) the chain conformations and free-volume distribution within the polymer canopy, (2) the dynamic relaxation behavior of the polymer canopy, and (3) the number of polymer entanglements between canopies of nearby PGNs. The first will allow validation of theory and/or coarse grained simulations versus existing experimental results, while the latter two are important in determining the plasticity and toughness of these systems.

5. **Description:** Polymer-grafted nanoparticles are a class of inorganic-organic nanocomposites in which the volume fraction and spacing of the inorganic constituent can be precisely tuned by adjusting the length and grafting density of the tethered polymer. This additional constraint on polymer conformations due to the end-tethering of the chains has substantial impact on fundamental properties, including free-volume, viscosity, toughness, and electro-optic characteristics, such as dielectric breakdown and optical scattering. For example, PGNs 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, optical, and energy storage properties.

   The connection between the architecture of the PGN (e.g. experimentally controllable parameters of graft density, graft length, and nanoparticle size), the properties of the supporting surface, and the resulting interparticle spacing and film properties must be made clear to allow for rational design of PGNs for such technologies. This effort will use theory and/or coarse grained simulations to reveal the polymer conformations, entanglement network, and local dynamics of PGNs on surfaces as a function of their architecture. Also of interest is a prediction of how solvent swelling or a densely grafted polymer brush on the substrate alter the transport through and order within PGN assemblies. Fundamental insights gained regarding PGNs will build on the existing knowledge of the behavior of linear chains, dendrimers, and block-copolymers on surfaces; and thereby this work will develop a broader understanding of how molecular-scale architecture impacts the behavior of ultra-thin nanocomposite 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