RX20-28

1. **Research Title:** 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)

4. **Objectives:** Through theory, simulations, and/or synthesis develop a macromolecular-level understanding of the behavior of assemblies of polymer-grafted nanoparticles (PGN) with interpenetrating canopies. Of special interest is an understanding 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. Such insight will allow improved PGN design through the incorporation of secondary interactions (e.g. hydrogen boning, metal chelation, ionomer clusters, etc.) into the canopy to enhance plasticity, toughness and transport.

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 print applications, as green bodies for high-performance ceramics, as protection coatings for kinetic survivability, or as films within optical or energy storage devices.

   The connection between the architecture of the PGN (e.g. graft density, graft length, graft composition, nanoparticle size, nanoparticle shape), the process history, 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, simulations, and/or synthesis to reveal how PGN architecture influences local polymer conformations, interparticle entanglement, distribution of secondary interactions with the canopy, and multiscale dynamics on surfaces and within their 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 affects the behavior of ultra-thin nanocomposite films. These insights will guide future experimental work in constructing well ordered, reproducible, and mechanically robust arrays of particles for use in specialty printing, survivability, optical devices, or other applications.

6. **Research Classification/Restrictions:** Unrestricted

7. **Eligible Research Institutions:** Unrestricted