1. **Research Title:** Physics and Machine Learning for Polymer Materials Design
2. **Individual Sponsor:**

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3. **Academic Area/Field and Education Level**

   Chemical Engineering, Materials Science, Physics, Computer Science, Machine Learning, or related fields.

4. **Objectives:** Develop and test data-driven machine learning and/or physics-based models for accelerating polymer materials design

5. **Description:** Polymers are widely used in various technological applications for air and space. These materials are often processed, synthesized, or designed in a solution, where the resulting material performance depends on the solvent quality, viscosity, experimental conditions (e.g. temperature, pressure, etc.), polymer chemistry and kinetics, among other factors. Much of our understanding of how these processes affect macroscopic design is limited, and the ability to predict polymer solution properties such as their dynamics, self-assembly, and phase behavior is crucial to controlling morphology and structure. Artificial intelligence (AI) and machine learning (ML) models are accelerating the pace of R&D in materials science, but these methods often require sufficient quality data which is a challenge. This research aims to integrate physics-informed machine learning models to elucidate the effect of polymer chemistry, architecture, processing conditions, and other thermodynamic variables on the equilibrium and nonequilibrium behavior of polymer melts and solutions. Key interests include the self-assembled structure, morphology, phase behavior, rheology, and/or dynamics of high-temperature polyimides, polyelectrolytes, dynamic networks/vitrimers, nanocomposites, and sequence-based or complex-shaped polymers. Techniques include regression and classification machine learning, molecular dynamics simulations, and high-throughput experimentation/modeling methods for accelerating data availability.

6. **Research Classification/Restrictions:** Unclassified and unrestricted
7. **Eligible Research Institutions:** Any
8. **PA Approval #:** AFRL-2025-4009

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