1. Research Title: Understanding onset of damage in multifunctional vitrimer nanocomposite

## 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

- Develop hierarchical vitrimer -based multifunctional nanocomposites.
- Understand the onset of damage in multifunctional self-healing composites.
- Conduct nanoscale strain and damage mapping.
- Develop methods to monitor local healing of cracks.
- Uncover processing—structure—property relationships using a combination of experimental and computational methods.

#### 5. Description

The design of efficient multifunctional composites hinges on two pillars: intelligent materials engineering and advanced damage prediction tools. Nature provides compelling examples of composites that combine high toughness with strength, offering valuable inspiration for synthetic systems. However, natural materials still surpass many engineered counterparts, particularly in their resistance to damage and failure.

One of the key challenges in this domain is gaining a mechanistic understanding of failure processes. Specifically, we seek to elucidate how nanofiller characteristics—such as size, shape, orientation, and interphase morphology—influence damage initiation and progression in vitrimer nanocomposite. The chemical and microstructural nature of the interphase plays a critical role in defining composite behavior, yet remains poorly understood.

Our research takes a comprehensive, multidisciplinary approach that integrates synthesis, processing, multi-scale experimental characterization, and computational modeling to address these fundamental questions. By doing so, we aim to build a predictive understanding of failure mechanisms spanning from the nanoscale to the macroscale.

#### **Key Focus Areas:**

- Nature-inspired design of hierarchical material architectures.
- Mechanistic insight into fracture processes governed by nanofiller chemistry, morphology, and distribution.

- Evaluation of coupled mechanical, thermal, electrical, and optical properties.
- Generation of datasets to inform and validate molecular dynamics and mesoscale mechanical models.

### **Techniques and Methodologies:**

- Controlled processing of hierarchical vitrimer nanocomposites incorporating low-dimensional materials.
- Bulk and surface spectroscopy for chemical analysis.
- Thermo-mechanical testing for structure-property correlation.
- High-resolution X-ray micro–computed tomography ( $\mu$ CT) for 3D damage and structural visualization.
- Nanoscale mapping of chemical, physical, and mechanical properties.
- Advanced microscopy (AFM, SEM, TEM) and in-situ mechanical testing.
- Multi-scale computational modeling to simulate and predict material behavior.
  This integrated approach will ultimately inform the rational design of multifunctional, damage-tolerant, self-healing composites with tailored properties for high-performance applications.
- **6. Research Classification/Restrictions:** Unrestricted
- 7. Eligible Research Institutions:

**DAGSI** (Wright State University, AFIT, Ohio State University, University of Dayton, Miami University, Ohio University, University of Cincinnati)

8. PA Approval #: AFRL-2025-3683