RX21-31

1. **Research Title:** Stochastic Modeling of Thermoset Curing towards Correlating Molecular Structure with Transient Cure Properties

2. **Individual Sponsor:**

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

4. **Objectives:** To develop and employ a stochastic curing scheme for quantitative mapping between molecular structure of polymeric resins and transient thermo-physical properties during their cure process.

5. **Description:** Polymeric matrix composites (PMCs) have been one of the major cornerstones towards manufacturing customized aerospace components for decades, geared towards a variety of applications. With ever-changing focus towards lighter and superior composites, there is a continual need for exploring novel resin chemistries. Here, identifying an optimal cure cycle for a new resin via a conventional approach requires a great amount of research effort involving running several cure cycles for different degrees of curing (a vast parameter space in time and temperature) as well as follow-up characterization to measure various thermo-physical properties (degree of cure, glass transition temperature, moduli, residual stresses, etc.). In a similar context, while *in-situ* monitoring of such properties during cure (e.g. additive manufacturing) provide a valuable tool towards transient behavior of resin properties under cure, these tools are still in their early stages and are a growing area of active research. This work will model the network growth process via stochastic routes (well associated with events during experiments) providing an alternative and more cost-effective means to address and approach a better understanding of cure dynamics and pinpoint transient properties associated with cure reactions. The detailed chemistry of initial reactants will be captured at a coarse-grained level via their relative molecular masses, while the reaction specifics (rates, exotherm/endotherm) will be obtained via quantum mechanics and will be used as an input in the stochastic model. A coarse-grained network growth model based on stochastic dynamics is capable of capturing spatial and temporal timescales and events and hence provide a better understanding of curing processes and transients over several length scales. It is expected that this framework enables identification of resin systems that are required to stay within experimental bounds of their transient properties (such as heat of reaction, max reaction temperature, polymerization stresses).

6. **Research Classification/Restrictions:** This research has no ITAR restrictions.

7. **Eligible Research Institutions:** Place an X in all that apply.

   X Universities (DAGSI) X AFIT (only) X USAFA

8. **Interest in Summer USAFA Cadet: Yes**