RX21-30

1. **Research Title:** Using Machine-Learning and Data-Analytics for Exploring Low-Density Materials for High-Temperature Thermo-Oxidative Stability.

2. **Individual Sponsor:**

Dr. Vikas Varshney, AFRL/RXCCP
AFRL/RXCC Bldg. 655 / Room 023
2230 Tenth Street
WPAFB, OH 45433-7750
vikas.varshney.2@us.af.mil

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, employ and validate a machine-learning framework for identifying novel low-density materials which possess high thermal oxidative stability. A number of quantum calculations as well as data analytics on molecular descriptors will be carried out towards identifying molecular as well as elemental signatures which correlate with increased thermal stability.

5. **Description:** Currently, metals/ceramics and their alloys dominate the materials selection criteria for development of high-temperature (>1000 °C) aerospace components because of their high temperature stability as well as resistance for degradation/fatigue by various environmental factors. As most of the metal/ceramic-based components are of high density, there exists an opportunity for weight-associated cost-reduction in exploring low-density materials (such as organic polymers) as well as their composites that offer high temperature stability. Using polymeric matrices based composites (PMCs) also provide better flexibility and modularity in structural and multi-functional design-space. Current state-of-the-art high-temperature PMCs possess operational temperatures of ~330 °C, and hence, presents a large elevated-temperature design space (up to 600 °C) to be explored via intelligent selection of high-temperature stable polymeric constituents. In this work, we plan to use and machine learning frameworks similar to QSAR (quantitative structure-activity relationships) methods to select potential molecular entities that offer high temperature stability via exploring several types of topological and geometric molecular descriptors. Thereafter, quantum chemical calculations on the newly postulated molecular compounds based on these key molecular entities will performed in order to calculate transition-state activation energies for defragmentation (breaking or degradation) for further validation of the machine learning framework. This work will provide a scientific guidance to experimentalists for the experimental realization of the better thermally stable PMCs.

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**