RX19-24

AFRL RESEARCH TOPIC CALL FOR FY19

1. **Research Title:** Screening Low-Density Materials for High-Temperature Thermo-oxidative Stability via Machine Learning Algorithms

2. **Individual Sponsor:**

Dr. Vikas Varshney, AFRL/RXCCP
AFRL/RXCC Bldg. 655 / Room 013
2230 Tenth Street
WPAFB, OH 45433-7750
vikas.varshney.1.ctr@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 machine learning framework for identifying potential low-density materials which possess high thermal oxidative stability. A number of quantum calculations are to 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 integrate computational chemistry findings with machine learning framework to select potential molecular entities that offer high temperature stability. Here, we plan to use commercial off-the-shelf (COTS) computational chemistry packages to calculate transition-state activation energies for defragmentation (breaking or degradation) of a plethora of molecular candidates with diverse set of organic and/or organic/inorganic hybrid features. Thereafter, SMILES notation based molecular descriptors will be employed to correlate molecular features with activation energies and help identify molecular signatures that can lead to higher thermal stability and 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) ☐ AFIT (only) ☐ USAFA

8. **Interest in Summer USAFA Cadet: No**