Attachment 1 - Research Topic Template

1. **Research Title:** Resin/fiber interphase characterization for polymer matrix structural composites.

2. Individual Sponsor:

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- 3. Academic Area/Field and Education Level: Materials Science and Engineering, Mechanical Engineering, Chemical Engineering, or equivalent (M.S. level)
- 4. **Objectives:** The goal of this effort is to better understand the chemical bases for resin/fiber interphase mechanical properties. The objectives are to attain this by 1) simulating the atomistic diffusion and curing reactions associated with sizing agents, resin, and the fiber surface for a thermoset polymer composite system, 2) exploring the effects of curing conditions on cross-linked network development and binding to the fiber surface, and 3) estimating the elastic behavior of the polymer/resin interphase.
- 5. Description: Qualification and certification of polymer composite materials and structures is a major initiative within the Air Force, specifically within the Air Force Research Laboratory. In addition, the aim is that component design will include materials design (rather than constraint to a limited number of established material choices). Future needs of Air Force systems impose ever-increasing demands on material properties and also impose stringent requirements on the time line and cost of their insertion. The long-range goal is to enable virtual design of material systems from constituent properties in the framework of integrated structural design, where material and structure definitions are essentially merged.

The fiber/matrix juncture plays a key role in determining composite toughness and other mechanical properties. Significant effort is devoted to its proper design. It is common to precoat fibers with agents (termed sizings) to ease handling and processing. These agents can also be used to tailor fiber/matrix bond integrity and enhance composite properties. The margin between the bulk matrix and the fiber (termed the interphase) plays a strong role in determining the composite's flexibility and strength. Knowledge of the sizing formulation and its role in subsequent processing is therefore valuable.

Experimental techniques have provided some insight into interphase chemical structure and mechanical properties but, owing to the small length scales, the results have provided limited insight. Interphase models have been of four principal types: continuum, chemical kinetic, thermodynamic, and atomistic. Mechanical continuum models have treated the interphase as having a known thickness and stiffness which is either uniform or graded. The interphase has also been represented as elastic boundary elements to determine interface stresses and bulk moduli. In chemical kinetic and thermodynamic models, the rate constants for phenomena are assumed to be known. Owing to the presence of a solid surface (and therefore the large spatial gradients in rates), these quantities are often challenging to determine by experiments.

Atomistic modeling to date has essentially ignored the existence of an interphase. While many have predicted adhesion energy, bulk stiffness, and "pull-out" strength of matrix thermoplastic or thermoset molecules near graphitic or ceramic surfaces, few have included surface-bonding agents. Highly pertinent questions yet to be answered include how kinetic interactions among surface, sizing, and resin functional groups as well as interdiffusion among resin and sizing species affect interphase dimensions and properties.

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5.	Research Classification/Restrictions: This research is unclassified.
7.	Eligible Research Institutions:
	DAGSI (Wright State University, AFIT, Ohio State University, University of Dayton, Miami University, Ohio University, University of Cincinnati) PA Approval #: 88ABW-2013-3602
	☐ AFIT (only)
	USAFA (only)
	If you are submitting a topic for the USAFA, please indicate if you are also interested in sponsoring a USAF Cadet in summer of 2013 (Avg Cost for USAF Cadet for 33 days was \$5000)
	Yes No D