SC EPSCoR

GEAR Collaborative Research Program (CRP)

SC EPSCoR Solicitation Number 8-CRP2019

Release Date: August 8, 2019; Updated: September 5, 2019

GEAR CRP Program Objectives

The goal of the GEAR CRP (Collaborative Research Program) is to encourage faculty researchers at the three South Carolina comprehensive research universities (CRUs), Clemson University, the Medical University of South Carolina, and the University of South Carolina; and predominately undergraduate institutions (PUIs) to build collaborative CRU/PUI academic research teams that will compete effectively for research funding. GEAR CRP grants will be awarded to build and enhance the network of scientists in the state that will conduct research related to the National Science Foundation (NSF) Research Infrastructure Improvement (RII) Track 1-Award entitled "***Materials Assembly and Design Excellence in South Carolina" MADE in SC***. The vision of the ***MADE in SC*** initiative is to discover and establish new and sustainable approaches for the design and assembly of hierarchical materials at multiple relevant length scales that service South Carolina's STEM research, education, and workforce needs and invigorate economic development. The focus of this initiative is to discover and develop new intelligently designed optical and magnetic materials, stimuli-responsive polymeric materials, and interactive biomaterials.

Proposals submitted in response to the GEAR CRP solicitation:

- must include two investigators with a senior faculty from a CRU and junior faculty from a PUI.
- **proposed research must be** collaborative, demonstrates a connection between experiments and Modeling and Computation Core (MCC) efforts (theory, computation, simulation, etc.), and be clearly aligned with the Materials Genome Initiative (MGI). ***This requirement was last updated on September 5, 2019.***

***MADE in SC* Research Priorities**

Proposals must respond to one of the following specific research thrusts. Proposals must address one or more of the activities listed in the Attachment titled, "List of Strategic Research Goals and Activities." The four research clusters of MADE in SC are:

1. **Modeling and Computation Core (MCC).** The goal of the MCC is to develop multiscale models and computational tools synthesizing theories, methods, and infrastructure to provide optimized solutions for the materials system. Supporting goals are the development of advanced multiscale theoretical foundations, fast algorithms to handle high throughput

computations, high resolution/fidelity imaging and visualization, and big data analytics including uncertainty quantification.

2. **Research Thrust 1 – Hierarchical Structures with Controlled Optical, Electrochemical, and Magnetic Properties.** The goal of Thrust 1 is to explore the inorganic crystal structure and mesoscale assembly of hybrid inorganic and organic materials to control and tailor their optical and magnetic properties. These designed materials and assemblies will exhibit multi-functional, correlated, collective properties leading to, e.g., materials for enhanced energy transfer for lasing and harvesting applications.
3. **Research Thrust 2 – Stimuli-Responsive Polymeric Materials.** The goal of Thrust 2 is to design and develop synthesis strategies for polymers able to respond to external cues leading to, e.g., materials for efficient water treatment and self-repairing materials for harsh environments.
4. **Research Thrust 3 – Rational Design of Interactive Biomaterials.** The goal of Thrust 3 is to develop a fundamental understanding of the effect of physical and chemical signals on cellular behavior across a range of length scales, leading to the development of interactive biomaterials, e.g., for use in regenerative medicine.

Award Information

Award Type: Grant

Maximum Funding Amount Per Project: $60,000.00

Project Duration: 12 months

Estimate Number of Awards: Depends on quality of proposals and availability of funds.

Anticipated Start Date: January 2020

Eligibility

- Faculty members from any South Carolina college or university may serve as a Principal Investigators.
- Current GEAR CRP PIs and GEAR PIs whose awards end before January 1, 2020 are eligible to apply and can serve as Co-PI.
- A GEAR CRP team must consist of at least one "mentor" faculty from a CRU, as PI or Co-PI, and one or more "target" faculty from one or more PUIs. **Mentor faculty members** are defined as those with tenure or tenure-track appointments at a CRU who are currently serving as the PI or Co-PIs on a major, peer reviewed and extramurally funded research project or who have served in that capacity within the past two years. **Target faculty members** are those who are in the formative part of their careers, still developing their research programs, and with a strong potential to obtain independent support. In some cases, a senior faculty member may be considered target faculty if the individual is entering a new field of research or is collaborating on a project outside of his/her discipline.
- Proposals that include target faculty from a Historically Black College or University (HBCU) are encouraged.

- Proposals that integrate modeling/simulations and experimental research are strongly encouraged.
- A minimum of two undergraduate students must be identified for participation in the project. Students must be enrolled as a STEM major at the home institution of the target faculty and must have high probability of matriculation into graduate school.
- Graduate student support is encouraged especially for students from underrepresented minority groups.
- The home institution of the PI will serve as the fiscal agent and will establish a sub-award for the institution of the Co-PI.

Deadline

Full Proposal – Monday, September 30, 2019 – 5:00PM EST

Full Proposal Content

The sections below represent the body of the proposal. Failure to submit the required sections will result in the proposal not being accepted or being returned without review. *Note: Where indicated, the number of pages refers to the maximum number of pages allowed and must not be exceeded.*

1. Cover Page (2 Pages)

Use the Cover Page form in Appendix A.

2. Project Summary (1 Page)

Proposals must contain an NSF compliant summary of the proposed project not more than one page in length. The Project Summary consists of an overview of the activities that would result if the proposal were funded, and a brief description of long-term plans for sustainability. It should specifically identify the MADE in SC research thrust areas and articulate the integration of modeling/simulations with experimental research. The Project Summary must also include a statement of objectives and methods to be employed, and two distinct sections: 1) statement on the intellectual merit of the proposed activity, and 2) a statement on the broader impacts of the proposed activity.

3. Project Description (8 Pages)

The Project Description should provide a clear statement of the work to be undertaken and must include the best scientific and strategic (long-term) objectives of the proposed work and expected significance, the relationship of this work to the present state of knowledge in the field, and the work plan. The Project Description section should have the following:

a. Objectives of the Proposed Work and Relevance

State the objectives of the proposed work and explain how it relates to ***MADE in SC*** research priorities outlined in the Program Objectives section. Proposers must identify the activity or activities that the proposal addresses from the "List of Strategic Research Goals and Activities" by specifying the Goal, Objective and the specific activity or activities.

b. Prior Relevant Research

Describe the proposed research project including significance of research and a review of relevant literature related to the proposed work.

c. General Research Plan

Describe the research framework, hypothesis, research questions, methods and procedures, potential outcomes, etc. Describe the broad design of activities to be undertaken (e.g., experimental methods and procedures). Proposers should address what they want to do, why they want to do it, how they plan to do it, how they will know if they succeed, and what benefits could accrue if the project is successful. The research activities may be based on previously established and/or innovative methods and approaches, but in either case must be well justified. These issues apply to both the technical aspects of the proposal and the way in which the project may make broader contributions. Proposers must clearly identify the accomplishments to be expected at the end of the project. Specific milestones must be carefully stated to aid in proposal evaluation.

d. Alignment with the Materials Genome Initiative (MGI) (*Section updated September 5, 2019*).

Describe the alignment of the proposed research with the Materials Genome Initiative (MGI) and explicitly identify how the proposed research connects with the MGI approach, i.e., an iterative cycle for materials design.

4. Mentoring Plan (2 Pages)

Describe the how the target faculty will be mentored. Examples include but not limited to: career counseling, grant proposal preparation, student mentoring skills, publications and presentations, research collaboration, etc.

5. Plans to Leverage GEAR CRP Funding (2 Pages)

Describe the plans to leverage GEAR CRP funding and explicitly address the targets and opportunities for future project funding and sustainability of the effort. Outline a plan for submitting research proposals to national and private funding agencies to attract research grants. The plan must include the names of potential agencies and the programs and dates (if known) that will be targeted.

6. References Cited

Reference information is required. Each reference must include the name of all authors (in same sequence in which they appear in the publication), the article and journal title, book title, volume number, page numbers, and year of publication.

7. Results from Prior SC EPSCoR Support (1 Page per Award)

The purpose of this section is to assist reviewers in assessing the quality of prior work conducted with current or prior SC EPSCoR Program funding. If any PI or Co-PI identified on the proposal has received a SC EPSCoR Program award as a PI since January 1, 2017, the following information must be provided:

- Title of the project, start date, date completed, and award amount.
- Summary of the results of the work completed, including accomplishments, supported by the award. The results must be separately described under two distinct headings: Intellectual Merit and Broader Impacts
- A listing of the publications resulting from the award (a complete bibliographic citation for each publication must be provided either in this section or in the References Cited section of the proposal); if none, state "No publications were produced from this award".

If the project was recently awarded and therefore no new results exist, briefly describe the proposed work.

8. Biographical Sketches (2 Pages per person)

A biographical sketch is required for the PI and the Co-PI(s). Biographical sketches of other senior personnel with whom the PI will collaborate may also be included. NSF format is required and must include and be limited to the following sections:

- **Professional Preparation** – undergraduate and graduate education and postdoctoral training (including location)
- **Appointments** – A list, in reverse chronological order, of all the individual's academic/professional appointments beginning with the current appointment.
- **Products** – A list of: (i) up to five products most closely related to the proposed project; and (ii) up to five other significant products, where or not related to the proposed project
- **Synergistic Activities** – A list of up to five examples that demonstrate the broader impact of the individual's professional and scholarly activities that focuses on the integration and transfer of knowledge as well as its creation.

For more information on NSF format, visit
https://www.nsf.gov/pubs/policydocs/pappg17_1/pappg_2.jsp#IIC2f

9. Budget

Use the Budget forms in Appendix B. If the PI and Co-PI are from two different institutions, two different budget sheets must be submitted; one for the PI and one for the Co-PI. The PI's budget sheet Section F must show the Co-PI's total budget amount as a subaward.

10. Budget Justification (2 Pages per institution)

The budget justification must be composed of no more than two pages for each institution and must include the following sections:

- Senior Personnel
- Other Personnel
- Fringe Benefits
- Materials and Supplies
- Equipment
- Domestic Travel Support
- Publication Costs
- Other Direct Costs

11. Current and Pending Support

The Principal Investigator and all senior personnel must complete Current and Pending Support document in Appendix C.

12. List of Conflicts

Provide conflicts of interest (COI) for each project participant on Appendix D. Conflicted individuals to be identified for each project participant include:

- PhD Advisor: PhD Advisor of the participant (a direct advisor, not simply a thesis committee member) at any time in the past
- PhD Advisee: PhD advisee of the participant (a direct advisee, not simply where student is on thesis committee) at any time in the past
- Co-author: a co-author of the participant (includes papers under review and in preparation) within the past 48 months
- Co-PI: a co-investigator of the participant (includes proposals under review and in preparation) within the past 48 months
- Postdoc Advisor: Postdoc Advisor of the participant (a direct advisor, not simply a collaborator) within the past 48 months
- Postdoc Advisee: Postdoc Advisee of the participant (a direct advisee, not simply a collaborator) within the past 48 months
- Collaborator: a collaborator other than those listed above within the past 48 months

(do not list individuals who have merely shared or received data, software, or other intellectual property)

- Co-editor: a co-editor of the participant during the past 24 months

Budget Information

Funding for the GEAR CRP Program is intended to support salaries and fringe benefits, materials and supplies, domestic travel support, publication costs, tuition supplement, etc.

- The budget requested may not exceed $60,000.00 per proposal.
- A maximum of one month of summer salary for the PI and/or Co-PI is allowed. No other senior personnel may receive funding from this program.
- Salary support is allowed for Post-docs, student researchers, and other staff.
- Indirect costs are not allowed under this solicitation.
- Cost-share is not required but encouraged.
- Awardees should ensure that costs claimed under SC EPSCoR Program grants are allowable, allocable, and reasonable.

Submission Instructions

PIs should submit their proposals via the SC EPSCoR Proposal Submission Portal at https://scepscoridea.org/Solicitations/portal/index.php. If not previously registered in the Portal, please follow the instructions on the main Portal page to register.

Proposal Review Process

Proposals that meet the eligibility requirements and the guidelines of this solicitation will be evaluated by external reviewers (outside South Carolina) based upon the extent to which they meet specific criteria including but not limited to:

- The potential of the proposed research to advance knowledge and understanding within the research priorities outlined in the Program Objectives section (Intellectual Merit).
- The potential for the proposed activity to benefit society, advance desired societal outcomes and broaden participation of groups that are under-represented based on gender, ethnicity, and disability (Broader Impacts).
- Whether the plan for carrying out the proposed activities is well-reasoned, well-organized, and based on a sound rationale, and whether it incorporates a mechanism to assess success.
- How well qualified is the PI/Co-PI team to conduct the proposed activities.
- The adequacy of available resources to carry out the proposed activities.
- How well does the proposed research integrates modeling/simulations with experiments?
- The likelihood that the research will lead to extramural funding.
- How well does the proposed activity advance discovery while promoting, mentoring, training, teaching, and learning?

Award and Reporting Requirements

- All GEAR CRP PIs and Co-PIs will be considered part of the MADE in SC Project and are expected to participate in MADE in SC activities which include attending meetings and contributing to the annual report submitted to the National Science Foundation (NSF).
- All publications (e.g., research publications, press releases, other publications or documents about the research funded by the SC EPSCoR Program) and presentations resulting from the GEAR CRP must include an acknowledgement of SC EPSCoR Program support and a disclaimer. "*Research reported in this [publication, press release, presentation] was supported in part by the NSF and SC EPSCoR Program under award number (NSF Award # OIA-1655740 and specific SC EPSCoR grant number). The views, perspective, and content do not necessarily represent the official views of the SC EPSCoR Program nor those of the NSF*."
- GEAR CRP Teams will be required to present their research findings at the SC EPSCoR and MADE in SC meetings.
- SC EPSCoR Program reserves the right to conduct site visits during the project period for evaluation and reporting purposes. Awardees are expected to provide required information and documentation to the SC EPSCoR Program staff and External Evaluator as needed.
- Reassurance of Responsible Conduct of Research (e.g., CITI Certification) are required for student researchers to be submitted to SC EPSCoR Program State Office.
- Progress reports are due every six months after the start date of the award. A template will be provided to the PIs.
- A final report will be due 60 days after the end of the award.

Contact Information

General inquiries regarding this program should be made to:

April Heyward, MRA
Program Manager, SC EPSCoR Program
T: 803.733.9068
E: april.heyward@scra.org

Attachment

List of Strategic Research Activities (Updated July 31, 2019)

MCC – Modeling and Computation Core

GOAL 1: Develop theories, computational tools and materials databases that complement experimental approaches for materials design and characterization using the MGI approach
Objective 1.a: Develop models and related algorithms in microscopic, mesoscopic, and macroscopic levels for various material systems
Activities
1. Develop theoretical and computational models for the thrust areas
2. Align modeling and simulation tools with specific needs in the materials thrusts
3. Integrate models with relevant experiments and validate the models through an iterative loop
Objective 1.b: Build comprehensive materials data structures to support data analytics and use of existing databases
Activities
1. Identify organizational structure best-suited for simulation and experimental data, compatible with existing materials database systems
2. Develop, implement, evaluate and refine web-based user interface for uploading and downloading data
3. Use established databases and share data with broader materials community
GOAL 2: Develop advanced computational tools that supports the framework for materials design and characterization
Objective 2.a: Implement visualization tools to enhance collaboration and link modeling and simulation with experiments
Activities
1. Identify connections that can be made between experimentalists and theorists that will facilitate simulation and visualization of experimental quantities at each scale
2. Develop improved visualization techniques and tools
3. Implement and distribute the tools in material design cycle
Objective 2.b: Implement modeling and simulation, data analytic and visualization tools in an optimized materials design and characterization framework
Activities
1. Design optimization through data acquisition, data mining, machine learning and uncertainty quantification techniques
2. Develop case studies for each thrust

Attachment

List of Strategic Research Activities (updated July 31, 2019)

Thrust 1 - Hierarchical structures with controlled optical, electrochemical and magnetic properties

GOAL 1: New structures with desired magnetic, electronic, and optical properties prepared via crystal growth
Objective 1.a: Synthesize and fully characterize new phases, including magnetic & luminescent oxides and fluorides
Activities
1. Data and simulation guided synthesize of complex iron and new rare earth containing oxides and fluorides and characterization of their magnetic and optical properties, respectively
2. Carry out chemical substitution reactions and optimize reaction conditions to target non-centrosymmetric space groups in order to investigate their magnetic and optical behaviors. Calculations will be carried out to guide material design and offer potential candidates
3. Characterize the ferroic behaviors and compositions with respect to their luminescence and upconversion behavior
Objective 1.b: Achieve the growth of mm sized crystals of promising magnetic, electronic, and optical materials from objective 1a.
Activities
1. Establish growth conditions that lead to crystals.
2. Refine methods to yield 0.5 mm sized crystals based on solubility/nucleation theory input. Theoretical models and calculations will be used to identify optimum conditions for growth of large crystals.
GOAL 2: Synthesis of uniform building blocks and new methods for building mesoscale assemblies
Objective 2.a: Synthesis of uniform organic and inorganic nanoscale hetero-structures
Activities
1. Utilize quantum chemistry-based prediction tools to develop candidate chemical structures and develop synthetic techniques for building blocks for mesoscale assemblies.
2. Characterize electronic, optical and magnetic properties and surface properties of building blocks as isolated and collective phase, compare results with simulations and if needed, refine simulations
Objective 2.b: Assembly of organic and inorganic nanoscale hetero-structures into mesoscale assemblies
Activities
1. Characterize optical, magnetic, and electrical and electrochemical properties of assembled hetero-structures
2. Convert building blocks into assembled 2D and 3D assembled structures. Use meso-scale simulations to design the assemblies
3. Utilize quantum chemistry-based prediction tools to develop candidate structures with enhanced intermolecular interactions which will allow for the design/synthesis of synergistic optoelectronic and magnetic properties through defect generation in isolated particles and collective systems; compare results with calculations and refine simulation models

Attachment

List of Strategic Research Activities (updated July 31, 2019)

Thrust 2 - Stimuli-responsive polymeric materials

GOAL 1: Develop new knowledge of how molecular components in materials and their interactions with the environment facilitate stimuli-responsiveness
Objective 1.a: Understand the role of molecular components in sensing/responsiveness and self-assembly
Activities
1. Develop theoretical models and simulation tools sensitive to stimuli-induced molecular changes
2. Synthesize second generation programmable polymers that are kinetically stable
3. Test binding and recognition properties
Objective 1.b: Define the role of copolymer topologies and macromolecular segments in stimuli-responsive and self-assembly materials
Activities
1. Develop and validate dissipative particle dynamics model for copolymer bottlebrushes using feedback from theory and simulations
2. Using MD predictions develop copolymers with segments that exhibit dynamic activity and self-healing
3. Feedback loop between simulations and experiments and polymer optimization
Objective 1.c: Understand molecular conformations that lead to self-healing
Activities
1. Develop mathematical models for predicting self-healing in polymers
2. Develop polymer-based composites with dynamic interfaces
3. Develop computational and optimization approaches for heterogeneous interfaces
GOAL 2: Understand how internal or external stimuli can be used to control new materials functions
Objective 2.a: Develop molecular sensors and understanding their role in new materials
Activities
1. Develop copolymer-based molecular sensors capable of responding to electromagnetic radiation
2. Understand kinetics and its role on stimuli-responsiveness and self-assembly
3. Model dynamics of responses
Objective 2.b: Develop new stimuli-responsive classes of materials capable of sensing
Activities
1. Develop equilibrium descriptors and kinetic theory on block copolymer micelles
2. Test diverse polymers and exp. conditions for effects on structure, nanoparticle distribution, micelle kinetics
3. Characterize structure and dynamics for theory validation
Objective 2.c. Develop dynamic characterization tools enabling time-sensitive measurements
Activities
1. Develop photo-responsive supra molecular polymers
2. Theoretical and computational modeling of dynamics of dispersed ferromagnetic nanoparticles in gels
3. Modeling and characterization of polymers/gel frequency responsiveness

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List of Strategic Research Activities (updated July 31, 2019)

GOAL 3: Develop new chemico-physical features in biomaterials that will lead to stimuli-responsiveness
Objective 3.a: Understanding of interactions between biological and synthetic polymers
Activities
1. Optimization of biohybrid polymersome formation
2. Develop prediction theories and computational methods for protein-polymer conjugates
Objective 3.b: Bio-inspired materials synthesis and development
Activities
1. Attach biologically active pendant groups to synthetic polymers
2. Characterize biological, chemical, physical properties

Attachment

List of Strategic Research Activities (updated July 31, 2019)

Thrust 3 - Rational design of interactive biomaterials

GOAL 1: Synthesis of representative polymeric biomaterials to support fabrication of customizable materials providing a range of chemical, physical and morphological properties.
Objective 1.a: Synthesize multifunctional polymers and polymeric assemblies as building blocks to modulate cellular response guided by simulations and data science
Activities
1. A quantitative model will be developed to describe small molecular ligands anchored to viral particles in order to guide modulation of cell–cell recognition
2. Synthesize polypyrrole/biopolymer composites
3. Synthesis of novel cationic antimicrobial polymers. Informed by an all-atom molecular dynamics simulations based on model anionic lipid membranes.
4. Synthesis of redox-active molecules and materials guided by genome mining methods
5. Develop data and simulation guided biocompatible polymers and polymer complexes
Objective 1.b: Prepare complex macromolecular or bio-macromolecular assemblies
Activities
1. Assemble virus and virus-like protein nanoparticles into structures guided by simulations
2. Synthesize conducting polymer/ biomaterial composite films and nanoparticles to control cellular adhesion and growth response. Use literature data and initial results to develop simulations
3. Controlling the co-assembly of polyester-based polymers with protein and protein-nanoparticles using simulations to predict interactions between synthetic polymers and protein building blocks
GOAL 2: 3D fabrication of biomaterial platforms featuring integrated micro and nano features to create controlled materials environments for interfacing with cells
Objective 2.a: Fabrication of base engineering structures with integrated micro and nano features
Activities
1. Develop and enhance 3D fabrication capabilities
2. Using simulation techniques, develop hypothetical 3D patterns for incorporation into biomaterials. Evaluate the cellular response to these novel patterns
3. Demonstrate surface modification of biopolymer composites through direct coupling of peptides and through the construction of brush-like structures using living polymerization reactions
GOAL 3: Determine how the biological functions of cells are influenced by their "materials environment"
Objective 3.a: Characterize the changes in the type, concentration, and distribution of receptors on cellular membranes as a direct response to how the cell perceives its environment
Activities
1. Characterize the interaction of cardiomyocytes and fibroblasts and their response to novel materials that promote regeneration of fibrotic phenotypes Provide data on these responses to MCC for inclusion in models.
2. Create a database of cell surface receptors and characteristics to understand and predict how cellular response can be controlled through ligand organization

Attachment

List of Strategic Research Activities (updated July 31, 2019)

Objective 3.b: Characterize cellular response and interactions with newly synthesized biomaterials
Activities
1. Characterize the response of cells to biomaterials and develop an iterative process using simulation tools to predict cell-material interactions
2. Identify and modify existing simulation tools to include interactions with biomaterials. Incorporate existing data to improve estimation of model parameters for cell-material interactions. Use this to guide development of materials
3. Design and fabricate prototype materials based on feedback from modelling and characterize the cell response to them.