SC EPSCoR/IDeA

***MADE in SC* Expected Year 1 and Year 2 Activities, Outcomes, and Outputs**

Modeling and Computation Core (MCC)

MCC Goals

- Goal 1 - Develop multiscale theories and materials databank that complement experimental approaches for materials design
- Goal 2 - Develop advanced computational tools and open source computational infrastructure that supports the materials design framework

MCC Expected Activities

- Develop multiscale theoretical and computational models for the thrust areas
- Align modeling and simulation tools with specific needs in the materials thrusts
- Identify organizational structure best-suited for simulation and experimental data, compatible with existing materials database systems
- Develop web-based user interface for uploading and downloading data
- Populate databank, use, and share data with broader materials community
- Identify what quantities, at each scale, should be visualized
- Develop multiscale visualization techniques and tools
- Build an interactive platform combining modeling and simulation, data, and visualization
- Design optimization through data mining, machine learning, and uncertainty quantification techniques
- Develop case studies for each thrust

MCC Expected Outcomes

- Novel and improved multiscale theories and computational tools for materials research
- Comprehensive virtual materials design framework synthesizing the database, modeling, and visualization
- Efficient and effective coupling of modeling and simulation with experimental research being conducted in this project

MCC Expected Outputs

- Papers and proposals, integrating theory/simulation with experimental research and accelerating advanced materials design
- Expandable and searchable database to facilitate materials research consistent with the prevailing data format

Research Thrust 1

Research Thrust 1 Goals

- Goal 1 – New structures with desired magnetic and optical properties prepared via crystal growth
- Goal 2 – Synthesis of uniform building blocks and new methods for building mesoscale assemblies

Research Thrust 1 Expected Activities

- Synthesize and characterize complex iron and new rare earth containing oxides and fluorides and characterize their magnetic and optical properties respectively
- Establish growth conditions that leads to crystals
- Develop techniques and particles with anisotropic surface modifications
- Utilize quantum chemistry based prediction tools to develop candidate chemical structures for particles
- Characterize surface properties of particles as isolated and collective phase
- Characterize magnetic and electrical properties of isolated particles and films
- Utilize quantum chemistry based prediction tools to develop candidate structures with enhanced inter-molecular interactions

Research Thrust 1 Expected Outcomes

- Development of new magnetic and photonic crystalline materials and new methods for building mesoscale assemblies
- Integration of the simulation tools with experimental research to efficiently guide the development of new materials and assemblies

Research Thrust 1 Expected Outputs

- New materials with unique optical or magnetic properties
- Increasing number of papers and proposals integrating theory/simulations and experimental research focusing on novel optical and magnetic materials

Research Thrust 2

Research Thrust 2 Goals

- Goal 1 – Develop new knowledge of how molecular components in materials and their interactions with the environment facilitate stimuli-responsiveness
- Goal 2 – Understand how internal or external stimuli can be used to control new materials functions
- Goal 3 – Develop new chemico-physical features in biomaterials that will lead to stimuli-responsiveness

Research Thrust 2 Expected Activities

- Synthesize mixed brush grafted nanoparticles for interfacial responsiveness
- Develop self-healing block copolymers containing responsive pendant side groups
- Synthesize copolymers with segments that exhibit responsiveness to biological environments
- Develop glucose-based copolymers with self-healing properties
- Synthesize and integrate inorganic nanoparticles with copolymers with self-healing characteristics
- Develop copolymer-based molecular sensors capable of responding to electromagnetic radiation
- Develop and understand the role of catalysts and coordination compounds in stimuli-responsive materials
- Develop experimental methods of measuring stimuli-responsiveness
- Develop variable response time capabilities in stimuli-responsive polymers
- Formulate new polymer synthetic methodologies leading to the development of bio-responsive sensors

Research Thrust 2 Expected Outcomes

- Development of new self-repairing materials and sensors
- Grafted nanoparticles for interfacial responsiveness as well as modeling of effects on sensing/response to environment
- Theoretical models and simulation tools that lead to the development of responsive polymers

Research Thrust 2 Expected Outputs

- New self-repairing materials and sensors
- Number of peer-reviewed publications, seminars, and conference presentations in responsive polymers acknowledging *MADE in SC* increasing every year

<u>Research Thrust 3</u>

Research Thrust 3 Goals

- Goal 1 – Synthesis of representative polymeric biomaterials to support fabrication of customizable materials providing a range of chemical, physical, and morphological properties
- Goal 2 – 3D fabrication of biomaterial platforms featuring integrated micro and nano features for interfacing with cells
- Goal 3 – Determine how the biological functions of cells are influenced by their "materials environment"

Research Thrust 3 Expected Activities

- Purify and surface conjugate virus nanoparticles
- Synthesize polypyrrole/biopolymer composites
- Synthesize metal-containing polymers
- Synthesize polyester-based biocompatible polymers
- Assemble virus and virus-like protein nanoparticles into structures
- Synthesize surface-modified conducting polymer/biomaterial composite films and nanoparticles
- Develop and enhance 3D fabrication capabilities
- Demonstrate surface modification of biopolymer composites through direct coupling of peptides
- Characterize the response of microvascular endothelial cells and dermal fibroblasts to representative biomaterials
- Create a database of cell surface receptors and characteristics
- Create a database of cellular energy economy characteristics at the computational computing center

Research Thrust 3 Expected Outcomes

- Development of new biomaterials that communicate and interact with cells
- Integration of the simulation tools with experimental research to efficiently guide the development of new materials and assemblies

Research Thrust 3 Expected Outputs

- New responsive biomaterials
- Number of peer reviewed publications, seminars, and conference presentations in responsive biomaterials acknowledging *MADE in SC* increasing every year

Contact Information

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