Attachment
List of Research Activities by Research Cluster

Modeling and Computation Core (MCC)

GOAL 1: Develop multiscale theories and materials databank that complement experimental approaches for materials design
Objective 1.a: Develop multiscale models in microscopic, mesoscopic, and macroscopic levels
Activities
1. Develop multiscale theoretical and computational models for the thrust areas
2. Align modeling and simulation tools with specific needs in the materials thrusts
3. Integrate newly developed multiscale models with relevant experiments and validate the models through an iterative loop
Objective 1.b: Design and build a comprehensive Materials Data Bank to support data analytics
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. Populate databank, use and share data with broader materials community
GOAL 2: Develop advanced computational tools and open source computational infrastructure that supports the materials design framework
Objective 2.a: Develop and implement **visualization tools** to enhance collaboration and link modeling and simulation with experiments
Activities
1. Identify what quantities, at each scale, should be visualized
2. Develop multiscale visualization techniques and tools
3. Implement and distribute the tools in material design cycle
Objective 2.b: Implement modeling and simulation, data, and visualization tools in an optimized materials design framework
Activities
1. Build an interactive platform combining modeling and simulation, data, and visualization
2. Design optimization through data mining, machine learning and uncertainty quantification techniques
3. Develop case studies for each thrust

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Research Thrust 1 – Intelligently designed optical and magnetic materials

GOAL 1: New structures with desired magnetic and optical properties prepared via crystal growth
Objective 1.a: Synthesize and fully characterize new magnetic oxides and new luminescent oxides and fluorides
Activities
1. Synthesize and characterize complex iron and new rare earth containing oxides and fluorides and characterize their magnetic and optical properties, respectively
2. Carry out chemical substitution reactions to target a non-centrosymmetric space group and multi-photon optical behavior in modified rare earth containing oxides
3. Characterize the ferroic behaviors and multi-rare earth compositions with respect to their luminescence and upconversion behavior
4. Develop modeling to pursue new compositions with improved multiferroic and optical properties
Objective 1.b: Achieve the growth of mm sized crystals of promising magnetic 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
3. Develop theoretical models to optimize reaction conditions to yield mm sized crystals
GOAL 2: Synthesis of uniform building blocks and new methods for building mesoscale assemblies
Objective 2.a: Synthesis of uniform organic and inorganic hetero-structured nanoparticles
Activities
1. Develop techniques and particles with anisotropic surface modifications
2. Utilize quantum chemistry-based prediction tools to develop candidate chemical structures for particles
3. Characterize surface properties of particles as isolated and collective phase
4. Characterize optical properties with photo and X-ray excitation of isolated particles and films
Objective 2.b: Assembly of organic and inorganic hetero-structured nanoparticles into mesoscale assemblies
Activities
1. Characterize magnetic and electrical properties of isolated particles and films
2. Convert particle in assembled 2D and 3D assembled structures
3. Utilize quantum chemistry-based prediction tools to develop candidate structures with enhanced inter-molecular interactions

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Research 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
Activities
1. Synthesize mixed brush grafted nanoparticles for interfacial responsiveness using feedback from theory and simulations
2. Develop initial model for chain conformation effects on sensing/response to environment
3. Apply model of chain grafted surface
Objective 1.b: Define the role of copolymer topologies and macromolecular segments in stimuli-responsive materials
Activities
1. Develop self-healing block copolymers containing responsive pendant side groups using feedback from theory and simulations
2. Synthesize copolymers with segments that exhibit responsiveness to biological environments
3. Integrate experimental and theoretical results
Objective 1.c: Understand molecular conformations that lead to self-healing
Activities
1. Develop glucose-based copolymers with self-healing properties using feedback from theory and simulations
2. Synthesize and integrate inorganic nanoparticles with copolymers with self-healing characteristics
3. Develop computational approaches to 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 and understand the role of catalysts and coordination compounds in stimuli-responsive materials using feedback from theory and simulations
2. Develop experimental methods of measuring stimuli-responsiveness

3. Develop mesoscale computational methods integrated with collaborative EM/SAXS experimental facilities
Objective 2.c. Develop dynamic characterization tools enabling time-sensitive measurements
Activities
1. Develop variable response time capabilities in stimuli-responsive polymers
2. Develop mesoscale chemical imaging and visualization of kinetics of stimuli-responsive processes
3. Model and experimentally measure transient effects in stimuli-responsiveness
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. Formulate new polymer synthetic methodologies leading to the development of bio-responsive sensors
2. Develop prediction theories and computational methods for sensors based on copolymer topology
Objective 3.b: Mimicking biological systems in new materials synthesis and development
Activities
1. Attach biologically active pendant groups to synthetic polymers
2. Conduct biological testing

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Research Thrust 3 – 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
Activities	
1.	Purify and surface conjugate virus nanoparticles
2.	Synthesize polypyrrole/biopolymer composites
3.	Synthesize metal-containing polymers
4.	Synthesize polyester-based biocompatible polymers
Objective 1.b:	Prepare complex macromolecular or bio-macromolecular assemblies
Activities	
1.	Assemble virus and virus-like protein nanoparticles into structures
2.	Synthesize surface-modified conducting polymer/ biomaterial composite films and nanoparticles
3.	Co-assemble polyester-based polymers with protein and protein-nanoparticles
GOAL 2:	**3D fabrication of biomaterial platforms featuring integrated micro and nano features 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.	Demonstrate growth and patterning ability for integrated micro and nano structures as cell-materials interfacing substrates
3.	Demonstrate surface modification of biopolymer composites through direct coupling of peptides
4.	Demonstrate surface modification of biopolymer composites 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 response of microvascular endothelial cells and dermal fibroblasts to representative biomaterials

2. Characterize the response of microvascular endothelial cells and dermal fibroblasts to engineered surfaces	
3. Create a database of cell surface receptors and characteristics	
Objective 3.b:	Characterize cellular energy economy and energy phenotype in response to interactions with newly synthesized biomaterials
Activities	
1. Characterize the response of microvascular endothelial cells and dermal fibroblasts to representative biomaterials	
2. Create a database of cellular energy economy characteristics at the computational computing center	
3. Design and fabricate prototype materials and characterize the cell response to them. Feed this information back to the MCC	