List of Strategic Research Activities

From MADE in SC Strategic Plan version 3 (October 7, 2019)

MCC – Modeling and Computation Core

GOAL 1: Develop theories and computational tools, at relevant length scales including multiscale, and materials data structures 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, including, where appropriate, integration at different 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
3. Share the tools with the materials design community

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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

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Thrust Area 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
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

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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
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.