Five Year Strategic Plan for:

LA-SiGMA

Louisiana Alliance for Simulation-Guided Materials Applications

National Science Foundation Cooperative Agreement EPS-1003897

PI/PD: Michael Khonsari

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Executive Summary

Louisiana proposes to transform research and education in computational materials science throughout the State by creating the **Louisiana Alliance for Simulation-Guided Materials Applications (LA-SiGMA**). The goal of this five-year project is to position the State to compete for and secure a federally funded center of excellence in materials science and engineering in Louisiana. We will accomplish this by leveraging existing statewide computational, experimental, and intellectual assets.

LA-SiGMA Mission:

The mission of LA-SiGMA is to establish a sustained national center of excellence in computational material science by the end of the project period.
To accomplish this mission, the Alliance will

a) *Make transformative advances in the areas of electronic materials, energy materials and biomolecular materials;*
b) *Develop multi-scale materials simulation tools that take advantage of emerging paradigms in computational science;*
c) *Build strong interdisciplinary and interinstitutional teams that overcome geographical separation through effective use of cyberinfrastructure;*
d) *Contribute to the development of a diverse and technically sophisticated workforce;*
e) *Engage a wide spectrum of the State's population through outreach efforts; and*
f) *Form sustainable partnerships with industry and national and international collaborators.*

LA-SiGMA Vision:

Transformative advances in materials science research and education through a sustained multidisciplinary and multi-institutional alliance of researchers.

Realizing the Vision:

The LA-SiGMA Research Roadmap shown on the next page focuses the intellectual, computational, and experimental assets of the State towards the realization of this vision.

The research program of LA-SiGMA will be structured around three Science Driver (SD) teams of experimentalists, theorists, and computational scientists. The membership of the SD teams will contribute to a "Computational Team" (CT) tasked with the development of formalisms for multiscale materials simulations relevant to all three Science Drivers. The CT will also include computational scientists who will help translate the formalisms into algorithms and codes that take advantage of current and anticipated high-performance computing platforms. The commonality of the tools is the "glue" that tightly integrates the three Science Drivers.

The main goals of the SD and CT teams are as follows:

Science Driver 1: Electronic and Magnetic Materials: *Transform the field by extending many-body formalisms and first principles methods to much larger length scales than currently possible.*

Science Driver 2: Materials for Energy Storage and Conversion: *Develop and apply multi-scale computational tools to study materials for energy generation, storage, and conversion.*

Science Driver 3: Biomolecular Materials: *Develop, apply, and experimentally validate multi-scale computational tools for the design of novel vehicles for drug delivery and other applications.*

Computational Team: *Develop multi-scale formalisms, algorithms, and codes for materials simulations and modeling; leverage existing tools and make optimum use of the next generation computing environments.*

Broader Impacts:

Strong education and training programs tightly integrated with the research program is essential to sustain and build on the accomplishments of the Alliance. Programs specifically aimed at increasing the diversity of the State's STEM workforce and those aimed at engaging and enlightening the public at large are also essential. Therefore, in addition to the research activities of the three science drivers (see LA-SiGMA Research Roadmap), LA-SiGMA will initiate, maintain, and evaluate additional activities under five key strategic directions (KSDs) whose goals are stated below.

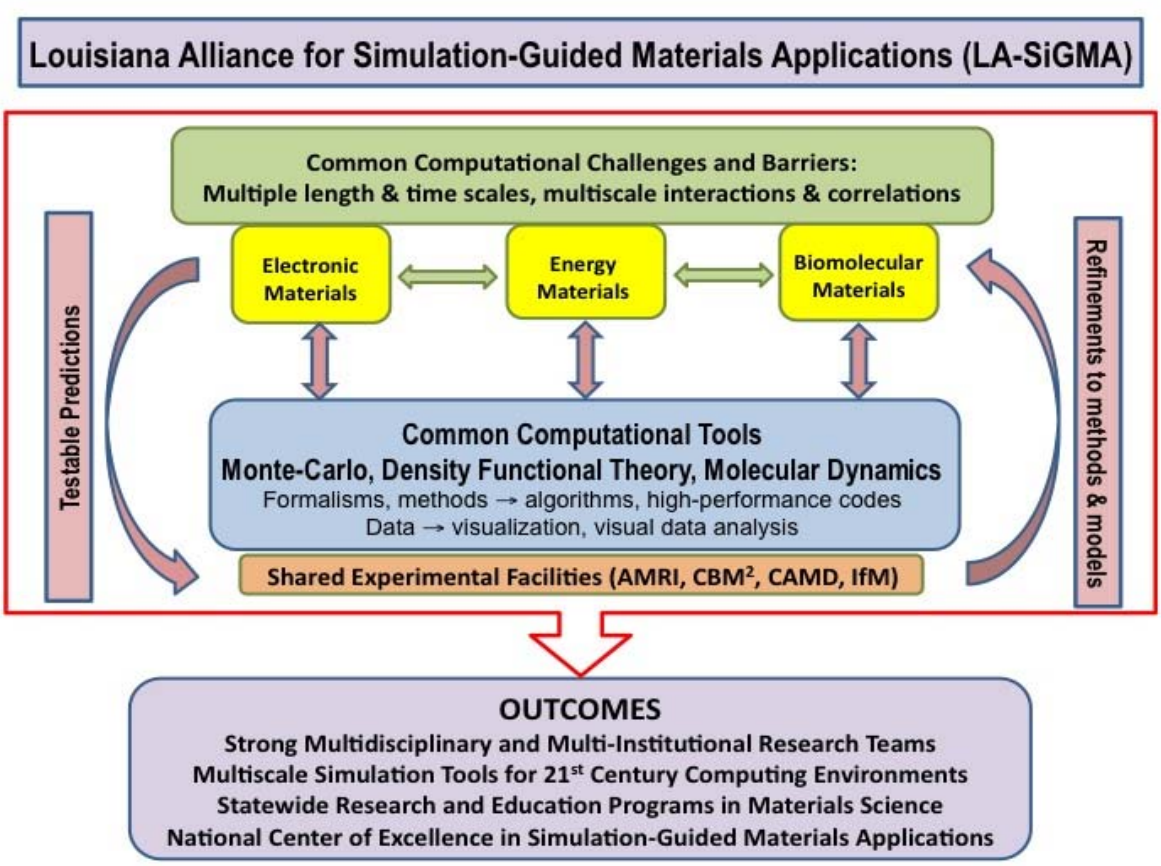
KSD 1. Diversity: *Dramatically increase the number of underrepresented minorities (URM) and women in the Alliance.*

KSD 2. Workforce development: *Address many levels of the educational ladder through training and educational activities.*

KSD 3. External engagement: *Utilize a multiplicity of methods to engage researchers, K-12, community colleges, industry, and the general public.*

KSD 4. Sustainability-Research Infrastructure: *Compete effectively for an NSF-funded Center of Excellence in Materials Science Research & Education.*

KSD 5. Sustainability-Faculty Development: *Initiate and implement programs designed to propel Louisiana faculty to national competitiveness.*



LA-SiGMA Research roadmap. Common challenges and barriers (green) link three science drivers (yellow) of scientific and technological importance that leverage existing strengths in the State. Common computational tools will be developed and implemented on the next generation of high-performance computing plat-forms (blue). Experiments at existing facilities (orange) will test computational predictions and lead to refinement of forma-lisms. These collaborative activities will lead to transformative advances in materials science research and education in the State.

Introduction

On October 1, 2010, NSF awarded Louisiana EPSCoR a five year, $25M Research Infrastructure Improvement (RII) Award for computational materials science in Louisiana. With the funds, Louisiana has created the Louisiana Alliance for Simulation-Guided Materials Applications – LA-SiGMA. The Alliance represents a statewide research and education program focusing on correlated electronic materials, energy materials, and biomolecular materials. Within the overall theme of "computational materials science," these science drivers emerged as clear areas of strength through a statewide solicitation that yielded over fifty multi-institutional whitepapers from teams of researchers. The majority of these teams included computational and experimental researchers, providing a strong foundation for the proposed research program that relies on close collaboration between theorists, computational scientists, and experimentalists. A proposal to the National Science Foundation in response to the EPSCoR RII Track 1 solicitation was developed on this foundation during February-October of 2009. The funding of this proposal led to the creation of LA-SiGMA.

The Alliance capitalizes on the jurisdiction's Cyberinfrastructure (CI) and past investments in experimental and computational materials science. Program objectives include: building the next generation of experimentally validated formalisms, algorithms, and codes for multiscale materials simulations; implementing them on present and next generation supercomputers; and educating the next generation of a highly skilled workforce of materials scientists and engineers. The value added by these efforts is a major transformation of education, research, and workforce development in the State with strong multi-institutional partnerships brought together to integrate:

- An education plan that includes new materials science graduate courses delivered across the State;
- Well-developed relationships between research universities, two-year colleges, and the K-12 community through ongoing outreach efforts;
- Strong partnerships between Historically Black Colleges and Universities (HBCUs), two-year colleges, and other universities in the State;
- Involvement of predominantly undergraduate institutions as partners in research;
- A team focused on training students and researchers to fully utilize the next generation cyberinfrastructure (CI);
- Multifaceted diversity, workforce development, and external engagement plans including relationships with industries through researchers, industry liaisons, and the State EPSCoR Committee; and
- Rigorous evaluation and assessment by an external evaluator, and feedback through an External Review Board (ERB) to ensure that goals and objectives of the project are met.

Development of the Strategic Plan

A strategic planning meeting for LA-SiGMA was held on December 15 in the office of the Louisiana Board of Regents which accommodate the State's EPSCoR program. The meeting was attended by several members of the Louisiana EPSCoR Committee including the State's EPSCoR Director and PI of the RII proposal, Dr. Michael Khonsari, Co-PI's of the RII proposal, members of the LA-SiGMA Project Execution Team, Science Driver leads, the Computational Team lead, and leaders of the five Key Strategic Directions that represent the broader impacts of the project. The NSF EPSCoR program officer at that time, Dr. Maija Kukla was present at the meeting and contributed to the discussions. The meeting was facilitated by Drs. Cindi Dunn and Jan Middendorf of the Office of Educational Innovation and Evaluation at Kansas State University.

During the meeting, the framework for the LA-SiGMA strategic plan was established. The essential strategies, activities, expected outcomes, and evaluation metrics for each aspect of the project were discussed in depth among the project personnel. The strategic plan developed was refined in the days that followed, and submitted to NSF Feedback was received on June 17, 2011 and the plan was further revised. This document is the latest version. The strategic planning document will be periodically reviewed by the Project Execution Team and the EPSCoR Chair and Vice-Chair, and revised as needed. Changes to the plan will be reported to NSF as directed in the Strategic Plan Guidance document provided by NSF.

Document Organization

The plan is organized for ease-of-use by project participants, NSF, stakeholders, and other interested audiences. Project information can be found at the LA-SiGMA website: http://institute.loni.org/lasigma or by contacting Dr. Michael Khonsari, LA EPSCoR Project Director, Associate Commissioner for Sponsored Programs, Research and Development, Louisiana Board of Regents, 1201 North Third Street, Suite 200, Baton Rouge, LA (E-mail: michael.khonsari@la.gov, Phone: 225-342-4253)

LA-SiGMA Research Program

The research program of LA-SiGMA will be structured around three Science Driver (SD) teams of experimentalists, theorists, and computational scientists (see the road map figure in the Executive Summary). The membership of the SD teams will contribute to a "Computational Team" (CT) tasked with the development of formalisms for multiscale materials simulations relevant to all three Science Drivers. The CT will also include computational scientists who will help translate the formalisms into algorithms and codes that take advantage of current and anticipated high-performance computing platforms. The commonality of the tools is the "glue" that tightly integrates the three Science Drivers. The Science Driver teams will use these tools to generate testable predictions for systems of great scientific and technological importance. These predictions will be validated by experimentalists on the Science Driver teams, making use of existing materials research facilities in the State, and thus leverage the enormous investments already made. The close interactions between the computational, theoretical, and experimental scientists will help refine and guide the experimental and computational efforts. The experimentally validated computational approaches will transform the utility of simulation-guided materials science.

Alignment with the State's Science and Technology (S&T) Plan

Fostering Innovation through Research in Science and Technology in Louisiana (FIRST Louisiana) is a statewide S&T plan that will guide institutional planning and provide a foundation for a comprehensive statewide approach to research, development and innovation. This framework will guide Louisiana's post-secondary education research community and industrial and public-sector partners to strategically increase research productivity and build capacity in areas of long-term importance to the State. The plan has been endorsed unanimously by senior research leaders at every major research university in the State and has been authorized by the Board of Regents.

The plan is guided by a vision that places higher education as the leader in driving the State's dynamic innovation economy through the advancement of science and technology research and education. It is built upon the basic and applied sciences that lay the foundation for sustained innovation. It leverages the State's investments in people, tools and ideas in targeted multi-disciplinary areas for enabling cutting-edge research and innovation, such as materials science and information technology and biotechnology, that can impact research competitiveness as well as existing and emerging industries. The plan includes strategies for enhanced national competitiveness in translational research domains that relate both to the enabling science areas and to state and federal priorities-such as energy, the environment, biomedicine, agriculture and the digital world. Strategies are also identified to enhance the competitiveness of existing industries in the State and to foster the growth of new and emerging industry sectors in cooperation with Louisiana Economic Development. To this end, LA-SiGMA is playing a major role in fulfilling the goals and objectives of FIRST.

FIRST Vision:

By 2025, Louisiana's universities will lead the State's dynamic innovation economy through the advancement of Science and Technology research and education.

LA-SiGMA Vision:

Transformative advances in materials science research and education through a sustained multidisciplinary and multi-institutional alliance of researchers.

LA-SiGMA Mission:

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f) *Form sustainable partnerships with industry and national and international collaborators.*

The following pages cover the various project areas of the RII project, providing descriptions, goals, metrics, and impacts. Risks involved in meeting the individual project area milestones will be handled as described in the section entitled "Risk Management and Mitigation Plan" on page 19.

Research: Science Drivers, Focus Areas, and Milestones

LA-SiGMA has three science drivers and multiple focus areas within each science driver, as shown below.

Science Driver 1: Electronic and Magnetic Materials:

Description: *This class of technologically useful materials have electronic and magnetic properties that are unusual and unpredictable. A significant outcome of this science driver collaboration will be the ability to accurately model strongly correlated materials on national leadership class supercomputers for the first time. These models would allow for the development of new devices with greatly enhanced performance and sensitivity, such as molecular magnets and organic semiconductors.*

Key partners: LSU, LA Tech, GSU, SUBR, Tulane, UNO, Xavier

Goal: *Transform the field by extending many-body formalisms and first principles methods to much larger length scales than currently possible.*

Metrics:

- Publications involving new LA-SiGMAcollaborations
- Invited talks at international conferences
- Number of citations of SD1 codes
- Codes ported to NLC facilities
- New proposals from multi-institutional teams
- GPL codes used for published research by other groups
- Adoption of new DFT functionals by other groups
- Gender and ethnic diversity of SD1 members (including students & post-docs)

Impacts:

- Allow researchers to accurately model and predict properties of strongly correlated materials on national leadership class supercomputers for the first time
- Open-access SD1 codes will be ported to national leadership supercomputers

<table>
<tr><th rowspan="2">SD-1: Electronic and Magnetic Materials</th><th colspan="5">SMART Objectives</th></tr>
<tr><th>Y1</th><th>Y2</th><th>Y3</th><th>Y4</th><th>Y5</th></tr>
<tr><td rowspan="4"><u>Focus 1:</u> Multiscale Methods for Strongly Correlated Materials</td><td colspan="2">Develop GPU accelerated QMC solvers for next-generation supercomputers</td><td></td><td></td><td></td></tr>
<tr><td colspan="3">Incorporate Hyper-GGA functionals into common DFT codes including VASP</td><td></td><td></td></tr>
<tr><td></td><td colspan="3">Develop MSMB solver able to treat multiple correlated orbitals</td><td></td></tr>
<tr><td></td><td></td><td colspan="3">Port hyperparallel codes to NSF national leadership class machines (Blue Waters)</td></tr>
<tr><td rowspan="2">Focus 2: Correlated Organic and Ferroelectric Materials</td><td colspan="2">Test array of DFT functionals' prediction of metalloporphyrin and ferroelectric properties</td><td></td><td></td><td></td></tr>
<tr><td colspan="2">Prepare and measure electrical/magnetic properties of metalloporphyrin</td><td></td><td></td><td></td></tr>
</table>

		Develop experimentally validated computational models for porphyrin systems using magnetoresistance and electrical conductance measurements as guides		
			Develop multiscale models of metalloporphyrin systems using DFT parameters	
			Predict charge transport in metalloporphyrins and compare with experiments	
	Prepare organic magnets and ferroelectrics			
			Predict properties of ferroelectrics using new nonlocal meta-GGA DFT functional and GPU-accelerated simulations.	
		Investigate new opportunities in the simulation of batteries and basic processes essential to reduce chemical damage and increase energy density.		
Focus 3: Superconducting Materials	Address the bottlenecks and numerical instabilities in the parquet equations by employing better parallel linear systems solvers and develop multiband parquet codes			
	Incorporate Ramanujam's advanced tensor rotation and contraction methods (Tensor Contraction Engine) into parquet codes			
	Use hybrid QMC to address the origin of the QCP and competing order in cuprate models			
	Study overscreening in pnictide models using new Hyper-GGA functionals			
	Use methods that combine LDA models obtained from downfolding and DCA/MSMB to study correlation and phonon effects in the pnictides			

Science Driver 2: Materials for Energy Storage and Conversion:

Description: *The energy materials science driver will focus on the use of novel simulation methods to overcome the multiple time scales barriers in electrical storage materials, hydrogen fuels and catalytic reactions involving metal oxides. The resulting research will help the design of better electrochemical capacitors, fuel cells, hydrogen storage materials and metal oxide catalysts.*

Key partners: LSU, LA Tech, SUBR, Tulane, UNO

Goal: *Develop and apply multi-scale computational tools to study materials for energy generation, storage, and conversion.*

Metrics:

- Publications involving LA-SiGMA SD2 collaborations
- Invited talks at international conferences by SD2 members
- Number of citations to SD2 models and codes
- New proposals from multi-institutional teams
- SD2 Codes running on next generation computing environments
- Gender and ethnic diversity of SD2 members (including students & post-docs)

Impacts:

- Development of simulation tools that combine chemistry and physcis for the study of energy materials
- The discovery of improved materials for energy storage, generation, and conversion

SD-2: Materials for Energy Storage and Conversion	SMART Objectives				
	Y1	Y2	Y3	Y4	Y5
Focus 1: Electrochemical Capacitors and Fuel Cell Electrodes Based on Nanotube Forests	Conduct simulation of pore filling in electrochemical capacitors based on nanowire forests				
	Incorporate chemical processes in electrochemical simulations to study chemical damage at elevated electric potentials				
		Verify computationally the behavior of quantum capacitance in electrochemical capacitance			
			Explore additional nanoforest-based capacitor systems		
	Optimize computational efficiency of ab initio MD techniques				
		Predict catalytic sites in nanotubes			
			Design, build, and test fuel cells and use results to guide new calculations		
Focus 2: Thermodynamics and Kinetics in H2 Storage Systems	Extend the AVUS-HR, Gibbs, expanded ensemble methods to hydrogen in solids and locate spinodal points; calculate free energies of H_2 uptake in LiH_x (Y 1) and other storage materials (Y 2-5)				
	Use existing force fields (like ReaxFF) to calculate H2 uptake in bulk alloys (Y 1-2); develop new force fields for new and existing alloys (Y 2-5)				
		Investigate new opportunities in the simulation of batteries and basic processes essential to reduce chemical damage and increase energy density			
		Develop finite element model to track 3D microstructure evolution and finite difference models for ionic diffusion rates using distances			

		and times provided by experiments			
	Perform X-ray nanotomography imaging of H2 uptake in bulk alloys using Argonne's Advanced Photon Source (APS) (Y 1-2), and neutron tomography at NIST (Y 3-5)				
Focus 3: Catalytic Reactions Involving Metal Oxides	Develop force fields with environment-dependent charges for one metal oxide system				
	Perform computational modeling of water gas shift and Fischer-Tropsch reactions				
		Perform computational modeling of PCDD/PCDF production on metal oxide clusters			
			Develop new force fields and study of additional catalytic processes		
			Validate force field calculations with experimental measurements and DFT calculations		

Science Driver 3: Biomolecular Materials:

Description: *The goal of the biomolecular science driver is to develop novel biomolecular material systems, such as halloysite nanotubes, for the encapsulation, delivery, and release of therapeutics to targeted tissues.*

Key partners: LSU, LA Tech, GSU, Tulane, UNO

Goal: *Develop, apply, and validate experimentally multi-scale computational tools for the design of novel vehicles for drug delivery and other applications.*

Metrics

- Gender and ethnic diversity of SD3 members (including students & post-docs)
- Team publications, invited presentations, and proposals
- Interactions among multi-institutional teams
- Documented experimental validation of computational models
- Codes running on next generation computing environments

Impacts:

- Provide mechanistic insights into the assembly and synthesis of drug carriers
- Predictive computational tools for drug vehicles will be made available to the wider biomolecular materials communiity
- New interinstitutional/interdisciplinary collaborations will be built

SD-3: Biomolecular Materials	SMART Objectives				
	Y1	Y2	Y3	Y4	Y5
Focus 1: Unimolecular vehicles	Synthesize modular library of core molecules and amphiphilic side chains to explore encapsulation based on architecture and chemistry				
	Develop new inter-atomic interaction potentials and new coarse-grained force fields for systems containing both biological and nonbiological molecules				
	Develop new hybrid MD/continuum and coarse-grained and accelerated simulation strategies to link length and time scales in biological systems				
			Use multiscale methods to explore the role of architecture and solvent to optimize supramolecular vehicles for controlled capture and release		
Focus 2: Self-assembled delivery vehicles	Synthesize, characterize, and assess new transmembrane drug delivery systems				
			Experimentally utilize, validate, and ultimately improve the newly developed computational models for drug carriers, self-assembling, and translocation through bio-membranes		
		Use MD and CG methods to study the mechanisms of cellular absorption of drugs			
				Model new polymer architectures for new carriers, followed by synthesis in the laboratory	

Cyberinfrastructure:

Description: *The formalisms, algorithms and codes being developed in the LA-SiGMA project are being utilized jointly by all three Science Drivers. Therefore, a cybertools and cyberinfrastructure (CTCI) group has been assembled to allow Alliance members to more efficiently utilize the next generation of 21st-century supercomputers. CTCI includes members of all of computational and science driver teams.*

Key partners: LSU, LA Tech, SUBR, Tulane, UNO

Goal: *Greatly increase the impact of LA-SiGMA research and broader impact activities by leveraging existing cyberinfrastructure and facilitating the acquisition and optimal use of new technology.*

Metrics:

- Number of Research teams using and citing developed codes
- Number of LA-SiGMA codes running on National Leadership Class machines
- Number of LA-SiGMA codes developed for next-generation computers
- Successful follow-up cyber-related proposals
- Number of multi-institutional and multi-disciplinary advising and mentoring committees
- Placement of graduate students and postdocs

Impacts:

- Will contribute to a stong cyberinfrastructure for materials research and education
- A highly-trained compuational science workforce
- Successful migration to next-generation heterogeneous computers and National Leadership Class machines
- National and international use of LA-SiGMA software
- Broader use of visualization and workflow tools

Cyberinfrastructure	SMART Objectives				
	Y1	Y2	Y3	Y4	Y5
Leverage LONI facilities	At least 60% of the 4.5M SU's assigned to SD teams by 2nd quarter, 100% assigned by end of Y1				
Build on existing statewide software tools	All LA-SiGMA sites with HD video access by Y2		Twenty-five percent of SD researchers using common tools by Y5.		
Develop formalisms, algorithms, codes and expertise on next-generation computers and migrate to National Leadership Class computers	More than three codes developed for national leadership class machines by Y3				
Distribute and promote LA-SiGMA software through web portals	Four codes, with full documentation, publicly available by Y3				

Broader Impacts Key Strategic Directions:

Strong education and training programs tightly integrated to the research program is essential to sustain and build on the accomplishments of the Alliance. Programs specifically aimed at increasing the diversity of the State's STEM workforce and those aimed at engaging and enlightening the public at large are also essential. Therefore, in addition to the research activities of the three science drivers (see LA-SiGMA

Research Roadmap), LA-SiGMA will initiate, maintain, and evaluate additional activities under five key strategic directions (KSD) as outlined below.

KSD 1. Diversity

Description: *A variety of strategies designed to increase participation of women and underrepresented minorities (URM).*

Key Partners: *Institutions across the State*

Goal: *To dramatically increase the number of URM and women in the Alliance.*

Metrics:

- Documentation of the annual Meeting of the DAC with associated recommendations and follow-up
- The number and percentage of women and URM undergraduate and graduate students, faculty and post-docs participating in LA-SiGMA
- Number of women and URM students moving from 2-year institutions to 4-year colleges and to graduate school
- Number of graduate students and post-docs employed in academia, industry, and government laboratories

Impacts:

- Increased diversity in the Alliance
- Increased number of women and URM graduates
- Increased numbers of women and URMs employed in academia, industry, and gov't labs
- More 2-year students moving to 4-year institutions

Diversity Strategies	Milestones Y1	Milestones Y2-Y3	Milestones Y4-Y5
Establish a Diversity Advisory Council	DAC established in Y1	Annual DAC meetings	Annual DAC meetings
Provide financial incentives to women and URMs for pursuing advanced education and immerse in systemic mentoring environment	Establish program	Reach 30% women and 15% URM graduate students within the Alliance by Y3	Reach 40% women and 20% URM graduate students within the Alliance by Y5
Development of role models	Establish program	Reach 30% women and 15% URM graduate students within the Alliance by Y3	Reach 40% women and 20% URM graduate students within the Alliance by Y5
Create/expand pipelines to graduate school	Establish program	At least five students recruited through the pipelines described in the proposal by end of Y2	At least fifteen students recruited through the pipelines by end of Y5

for women and URMs			

KSD 2. Workforce development

Description: A comprehensive workforce development plan to contribute to a well-trained and diverse professional workforce that can support advanced materials research and industries as well as education.

Key Partners: *Institutions across the State*

Goal: *To address many levels of the educational ladder through training and educational activities.*

Metrics:

- Number of open house attendees
- Number of students in workshops
- Number of RET, REUparticipants
- Track Instructional changes implemented by RET teachers through follow-up visits
- Number of short courses
- Number of students enrolled in courses
- Number of industrial internships
- Participation in effective teaching workshops
- Track positions after graduation (industry, academia)

Impacts:

- Increased number of students in STEM careers in community colleges, undergraduate, graduate, and post-doctoral programs
- Increased exposure of middle- and high-school students to computational/materials science
- Engagement of community college students/faculty in STEM activities

Workforce Development Strategies	Milestones Y1	Milestones Y2-Y3	Milestones Y4-Y5
Open houses for middle and high school students and summer research workshops	100 open house attendees, and 40 students in summer workshops in Y1	Increased attendees in Y2-Y3	Increased attendees in Y4-Y5
RET programs for teachers	20 RET participants (as budgeted) each year; use of modules in classroom (tracked through follow-up visits to classrooms);	20 RET participants each year; expansion of pilot program	20RET participants each year
Multiple programs for two-year college students	Initiation of short-course pilot programs in Y1	Expansion of short courses in Y2 and beyond expansion of 2+2 programs to other LA-SiGMA institutions by Y3	Expansion of short courses and 2+2 programs.

REU programs on computational and experimental materials science	30 REU participants (as budgeted) each year; 50% of participants will pursue higher education	30 REU participants (as budgeted) each year; 50% of participants will pursue higher education	30 REU participants (as budgeted) each year; 50% of participants will pursue higher education
Distance Ed courses	Enrollments in new courses (at least 40 statewide)	Incorporation into graduate curricula on two campuses by Y2, others by Y3	Continued expansion of graduate curricula
Training programs for graduate students and postdocs	Participation in effective teaching workshops; five internships and extended visits each year	Participation in effective teaching workshops; five internships and extended visits each year	Participation in effective teaching workshops; five internships and extended visits each year

KSD 3. External engagement

Description: *Initiatives to inform and engage the general public in the activities of this transformative research and educational initiative.*

Key Partners: *Institutions across the State*

Goal: *To utilize a multiplicity of methods to engage researchers, K-12, community colleges, industry, and the general public.*

Metrics:

- Public lectures each quarter
- Web portal traffic, code downloads each year
- Number of international visits by faculty and students
- Industrial internships
- Number of NSF research highlights
- HD synchronous video usage
- Number of LA-SiGMAhighlights by LA-EPSCoRNewsletter
- Participation in bi-annual meetings
- International internships, proposals, presentations

Impacts:

- Increased public awareness
- Improved university-industry relations
- Dissemination of LA-SiGMA intellectual products
- Faculty who are better prepared to compete for federal funding
- Improved international collaborations and visibility
- Improved coordination among LA researchers

External Engagement Strategies	Milestones Y1	Milestones Y2-Y3	Milestones Y4-Y5
Communicate via public venues	At least one Louisiana Public Broadcasting (LPB) appearance per year by a LA-SiGMA	At least one LPB appearance per year by a LA-SiGMA member; at least one public lecture	At least one LPB appearance per year by a LA-SiGMA member; at least one public lecture

	member; at least one public lecture delivered each quarter; at least one lecture delivered to industrial audiences each quarter.	delivered each quarter; at least one lecture delivered to industrial audiences each quarter.	delivered each quarter; at least one lecture delivered to industrial audiences each quarter.
Web portals and social media offerings	Web portal created in Y1	Traffic increases 20% annually	Traffic increases 20% annually
Repository and versioning system	SVN created in Y1	SVN maintained and upgraded in Y2-5; 100 code downloads per year starting Y3	SVN maintained and upgraded in Y2-5; 100 code downloads per year
HD synchronous remote video	HD stations purchased and installed at participating institutions in Y1		
Brochures and newsletters	At least two LA-SiGMA highlights featured in LA EPSCoR newsletter each year; at least one story picked up by regional/national press	At least two LA-SiGMA highlights featured in LA EPSCoR newsletter each year; at least one story picked up by regional/national press	At least two LA-SiGMA highlights featured in LA EPSCoR newsletter each year; at least one story picked up by regional/national press
Formal mechanisms for communicating with NSF	Regular interactions with NSF; at least three research highlights reported to NSF annually	Regular interactions with NSF; at least three research highlights reported to NSF annually	Regular interactions with NSF; at least three research highlights reported to NSF annually
National, industrial, and international collaborations	At least one LA-SiGMA faculty and at least one student will visit and work in an international lab for one or more weeks each year	At least one LA-SiGMA faculty and at least one student will visit and work in an international lab for one or more weeks each year	At least one LA-SiGMA faculty and at least one student will visit and work in an international lab for one or more weeks each year

KSD 4. Sustainability-Research Infrastructure:

Description: Activities to leverage prior NSF EPSCoR investments and state-funded research facilities, to build statewide interdisciplinary research collaborations involving computational scientists, computer scientists and engineers, applied mathematicians, theorists, and experimentalists.

Key Partners: *Institutions across the State*

Goal: *To compete effectively for an NSF-funded Center of Excellence in Materials Science Research & Education.*

Metrics:

- Number of research team meetings with multi-institutional participation
- Team publications, invited presentations
- Composition of LA-SiGMA graduate committees
- Number of multi-PI proposals submitted and funded
- Number of research highlights from multi-institutional research

- Documented efforts to get PhD programs approved
- Number of courses delivered statewide by LA-SiGMAfaculty

Impacts:

- The development of multi-institutional research groups in each Science Driver area
- Increased funding success at the national level
- Increased collaborations

Sustainability – Research Infrastructure Strategies	Milestones Y1	Milestones Y2-Y3	Milestones Y4-Y5
Establish multi-institutional interdisciplinary research teams	60% of contributions to Y1 all-hands meeting will be from multi-university teams	Improvement in % of multi-university team contributions	100% of contributions will feature multi-university teams by Y5
Establish co-mentoring of students and postdocs	30% of graduate committees of students working for LA-SiGMA researchers will have members from another institution in Y1	Improvement in % of such committees	The percentage of such committees will increase to 70% by Y5
Enrich statewide materials science education with new courses and curricula	Planning activities	Proposals for new PhD programs (Materials Science and Engineering by LSU, UNO, and Southern; Molecular Sciences and Nanotechnology by LA Tech) submitted by Y2	

KSD5. Statewide Programs for Faculty and Student Development

Description: *A suite of statewide programs administered through the LA EPSCoR office that impact K-12, undergraduate and graduate students, post-docs, tenured and tenure-track faculty, and business and industry.*

Key Partners: *Institutions across the State,K-12 institutions business and industry*

Goal: *To provide programs designed to propel Louisiana faculty to long-term national competitiveness, and to encourage students to follow STEM careers. These programs are targeted to reach a wide audience across the State, and will be updated periodically to respond to changing needs.*

Metrics:

- Number of Peer reviewed publications associated with these programs
- Number and amount of proposals/new funding
- Number of Phase Zero grants that progress to Phase 1
- Number of Invited Presentations (target prestigious conferences)
- Number of presentations
- Number of faculty applying to the LA EPSCoR programs
- Survey results on impact of LA EPSCoR programs

Impacts:

- Increased collaboration in research
- Increased visibility of Louisiana faculty
- Enhanced national competitiveness of tenured and tenure-track faculty
- Greater opportunities for faculty education and training
- Increased agility of faculty to pursue new research ideas & cutting-edge techniques
- Enhanced industrial/academic partnerships
- More women and URMs entering the STEM 'pipeline'
- Increased exposure of K-12 students to science and engineering

Program	Milestones Y1	Milestones Y2-Y3	Milestones Y4-Y5
Pilot Funding for New Research (Pfund)	Award 45 Pfund projects	Award 40 Pfund projects per year	Award 40 Pfund projects in Y4 and 38 in Y5
Links with Industry and National Labs (LINK)	Fund 7 LINK visits	Fund 8 LINK visits per year	Fund 7 LINK visits in Y4 and 8 in Y5
Planning for Major Initiatives	Award 2 Planning Grants	Award 3 Planning Grants per year	Award 4 planning Grants per year
Opportunities for Partnerships in Technology with Industry (OPT-IN)	Award 8 OPT-IN projects	Award 8 OPT-IN projects per year	Award 8 OPT-IN projects per year
Travel Grants for Emerging Faculty (TGEF)	Fund 12 TGEF visits	Fund 12 TGEF visits per year	Fund 12 TGEF visits per year
Grantwriting Workshops	Fund 2 workshops per year	Fund 2 workshops per year	Fund 2 workshops per year
Supervised Undergraduate Research Experiences for URM (SURE)	Fund 20 research experiences	Fund 20 research experiences per year	Fund 20 research experiences per year
Speaking of Science Speaker's Bureau for K-12 (SoS)	Support 25 SoS presentations across the State	Support 25 SoS presentations per year	Support 25 SoS presentations per year

SBIR/STTR Phase Zero Initiative	Fund 12 Phase Zero projects	Fund 12 Phase Zero projects per year	Fund 12 Phase Zero projects per year

High Level Goals, Metrics, and Success Criteria for the Project:

RII Project Goal	Summative Metric	Success Criteria
Increase State's competitiveness for securing a federally funded national center of excellence in materials science through collaborative research	1. Success rate for federal proposals submitted 2. Major collaborative grants with interdisciplinary and interinstitutional researchers during RII 3. Accepted pre-proposals for centers during RII 4. Site visits for federally funded centers during RII	1. US average 2. 10 3. 4 4. 2
By the end of the RII project, Louisiana will succeed in establishing a federally funded center of excellence such as a MRSEC, NSEC, or STC.		
Increase focus of graduate education and training in the State on areas related to Materials Science	1. Statewide IGERT in Materials Science 2. NSF Graduate Fellowships secured by students working on Materials Science projects statewide	1. ≥ 1 2. ≥ 20
The RII project and related activities will establish a national model for collaborative graduate education and training in the area of Materials Science.		
Leverage CI and train workforce on the use of next generation high-performance computing environments	1. Research groups using toolkits and infrastructure developed by the "CyberTools" RII project 2. Codes ported to 21st-century computing environments	1. 25% 2. > 2 by Y3
The RII will develop new paradigms for effective collaboration between computer scientists and computational scientists while training young scientists to make effective use of the next generation of cyberinfrastructure for computation, data analysis, visualization, and communication.		
Strengthen relationships between State's universities and national labs and industries	1. Number of papers/conference proceedings resulting from graduate internships in industry or national laboratories each year 2. Industrial grants to support research in materials science to participating institutions during RII	1. > 5 2. ≥10
The RII will build the foundations for sustainable economic development in the State through mutually beneficial collaboration between academia and industry.		
Develop a highly trained workforce that sets national benchmarks in diversity.	1. 6-year graduation rate of women and minority graduate students participating in the project 2. REU students from 2-year colleges entering degree programs at 4-year institutions 3. Percentage of two-year college teachers in RET programs.	1. 100% 2. 25% 3. 15%
The RII will be transformative in increasing the number and diversity of students obtaining advanced training and advanced degrees in Materials Science and related areas		

Risk Management and Mitigation Plan:

Each project has a lead and co-lead. The science leads from each participating institution—all experienced scientists with the requisite management skills to lead large multidisciplinary projects—comprise the eight-member Project Execution Team (PET). The PET oversees the day-to-day activities of

the project and provides direction and guidance to project participants in each of the science driver and computational teams, and plays vital roles in ensuring effective communications between and within institutions. The project co-leads will assume leadership responsibilities to ensure a smooth succession of leadership, should it become necessary. At a minimum, the PET meets every other month with the PD and the Chair and Vice-Chair of the EPSCoR Committee. This process ensures that the project leadership is highly interconnected and aware of project activities. In the event of personnel departures or other unforeseen developments, PET members will be able to maintain project continuity.

Any major programmatic changes will be reviewed by the PET and brought to the attention of the ERB for their recommendations.

Given the tremendous current global interest and activity in all of the science driver and focus areas, there is high potential for unexpected and disruptive advances to be made in any of these areas. Therefore, the science driver teams will annually re-evaluate their research directions and milestones and would not hesitate to make adjustments as needed to maintain competitiveness and to remain at the frontiers of the research field.

Evaluation and Assessment:

A comprehensive Evaluation and Assessment (E&A) plan was created based on the research milestones, the success criteria for each strategy, and global metrics designed to measure the impact of the project on the jurisdiction's S&T enterprise.

The comprehensive plan, informed by current research and integrated into all program components, incorporates the following evaluation principles:

- **formative** evaluation to assess performance of project activities and provide feedback to improve the project and **summative** evaluation to assess and document the impacts and outcomes of the project;
- strategies to engage program participants in the evaluation process to obtain input from all stakeholders and ensure that the salient issues are captured and represented from multiple perspectives;
- employment of multiple research methods to triangulate data for more robust findings;
- application of multiple data collection methods (quantitative and qualitative) to assess the program's research, education, and outreach activities;
- development of various instruments including online questionnaires, annual site visits, observations, surveys[1] and focus groups/interviews[2] with faculty, staff, students and other project participants; and
- ongoing communication with Louisiana EPSCoR staff and participants.

The Evaluation & Assessment Team will execute this plan by providing raw data as well as summary evaluations to the External Review Board (ERB), which will guide and advise the Alliance. The execution of the plan will be based on (1) data collection, (2) data analysis, and (3) closing the loop by using the analysis results to make course corrections and improvements.

Data Collection: A web-based data collection system has been implemented to simplify the frequent data collection required for effective assessment of project activities. The LA-SiGMA researchers will provide the following metrics semiannually: (1) sharing of students, (2) sharing of postdocs, (3) participation in weekly seminars, (4) participation in summer programs and external engagement activities, (5) efforts in meeting the diversity goals set by the Alliance, (6) contribution to workforce training activities, (7) placement of students in industrial and national lab internships, (8) interdisciplinary and interinstitutional

[1] D. A. Dillman, J. D. Smyth, and L. M. Christian, *Internet, Mail and Mixed- Mode Surveys: The Tailored Design, 3rd Ed.* John Wiley, Hoboken, NJ, 2009.

[2] R. A. Krueger and M. A. Casey, *Focus Groups: A Practical Guide for Applied Research*. Sage Publications, Thousand Oaks, CA, 2000.

publications and presentations, (9) interinstitutional proposals, and (10) leveraging of RII funds by other funding sources. Each SD team will be expected to contribute to all aspects of the project, not just the scientific research. Data documenting implementation, impact, and effectiveness of all program components will be collected through a variety of mechanisms such as surveys, observation, document review, and interview/focus groups.

Data analysis: Quantitative and qualitative techniques are employed in the analysis. The raw data will be converted to a weighted score for each aspect of the project as well as for the Alliance as a whole. The relative weights and the scoring system are being designed in consultation with the external evaluator and statisticians to ensure that the scores are reliable success indicators.

Closing the loop: Feedback on their relative standing with respect to the stated goals and milestones established by the Alliance will be provided to every SD and KSD project team. The External Review Board, which will receive the raw data as well as the analysis, will confer with the Project Execution Team annually and provide recommendations. Course corrections will be made if specific project teams or a specific focus area appear to be falling behind. Examples of such corrections could include reassessment of project leadership or resources committed to the project. Standard methods will be used to analyze implementation, impact, and effectiveness data, and used in a similar manner.

Glossary

CI.....Cyberinfrastructure
CG.....Coarse-grained
CT.....Computational Team
DCA.....Dynamical Cluster Approximation
DFT .....Density Functional Theory
ERB.....External Review Board
FIRST.....Fostering Innovation through Research in Science and Technology (State S&T plan)
GGA .....Generalized Gradient Approximation
GSU.....Grambling State University
HBCU .....Historically Black College/University
HD .....High Definition
KSD.....Key Strategic Direction
LA Tech.....Louisiana Tech University
LINK .....Links with Industry, Research Centers, and National Labs (LA EPSCoR program)
LONI.....Louisiana Optical Network Initiative
LPB.....Louisiana Public Broadcasting
LSU .....Louisiana State University
MD.....Molecular Dynamics
MSMB.....Multiscale Many Body
OPT-IN .....Opportunities for Partnerships in Technology with Industry (LA EPSCoR program)
PCDD .....Polychlorinated Dibenzo-p-Dioxins
PCDF.....Polychlorinated Dibenzofurans
PET .....Project Execution Team
Pfund.....Pilot Funding for New Research (LA EPSCoR program)
QMC.....Quantum Monte Carlo
SD .....Science Driver
SoS.....Speaking of Science (LA EPSCoR program)
SMART.....Specific, Measurable, Actionable, Realistic, and Time-bound
SU .....Service Unit (LONI)
SURE .....Supervised Undergraduate Research Experiences (LA EPSCoR program)
TGEF.....Travel Grants for Emerging Faculty (LA EPSCoR program)
UNO .....University of New Orleans
URM .....Underrepresented Minority