Louisiana Alliance for Simulation-Guided Materials Applications (LA- SiGMA)

Leveraging Next Generation Supercomputing to Study Complex Emergent Phenomena in Novel Materials

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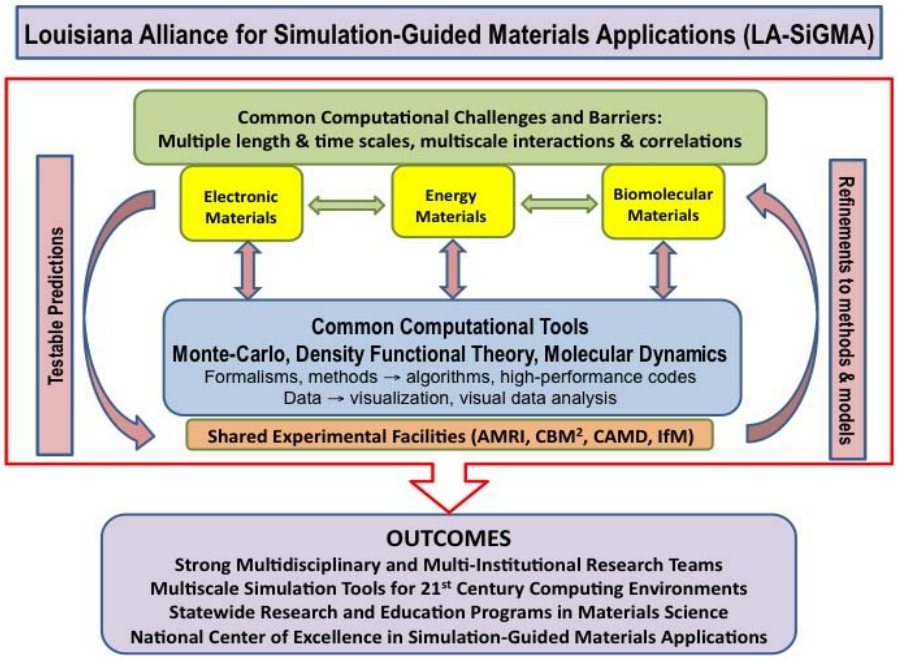
Project Summary

Many technologically important materials exhibit complex collective phenomena that cannot be predicted from the properties of the individual units. This behavior emerges due to correlations between the individual units spanning multiple time and length scales. This multiplicity of scales presents a formidable barrier to the simulation-guided design of modern materials. The scientific and technological challenges of addressing multiscale complex phenomena call for unprecedented collaboration of computational scientists, theorists, applied mathematicians, scientists, and engineers with expertise at each scale. They must take advantage of the enormous national investments in the next generation of hyperparallel, heterogeneous, multicore supercomputers to develop experimentally verified formalisms and algorithms that span all relevant scales. Developing collaborations that leverage new computational tools and experimental methods is both timely and prudent. According to NSF Director Arden Bement, we are on the cusp of a second Information Technology revolution "that may well usher in a new technological age that will dwarf, in sheer transformational scope and power, anything we have yet experienced in the current information age."* At the heart of this revolution is peer-to-peer collaboration, new modes of research and education, and virtual organizations that work across institutional boundaries. This is the premise of this proposal.

Intellectual Merit. We propose to transform materials science research and education throughout the State of Louisiana by creating the **Louisiana Alliance for Simulation-Guided Materials Applications (LA-SiGMA**). A major research focus of the Alliance will be to develop common computational tools for the study of multiscale phenomena in three Science Driver areas of current strength in the State, and of substantial technological and economic importance: **(1) correlated electronic materials, (2) energy materials,** and **(3) biomolecular materials**. The research roadmap for LA-SiGMA is shown in the accompanying figure.



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 platforms (blue). Experiments at existing facilities (orange) will test computational predictions and lead to refinement of formalisms. These collaborative activities will lead to transformative advances in materials science research and education in the State.

Rationale for the Proposed Research Program. Computational materials science is a relatively young field in which the capacity for discovery is largely driven by the development of new formalisms, algorithms, and codes. For example, density functionals with broad applicability (formalisms) developed by LA-SiGMA member John Perdew of Tulane, and associated implementation (algorithms) in widely-

* Cyberinfrastructure: The Second Revolution," Chronicle of Higher Education Jan 3, 2007, 53 (18) B5

used software packages have greatly increased the volume of research on the role of atomic and molecular clusters in catalysis and energy-related applications. The generalizations of dynamic mean field approximation developed by Mark Jarrell of LSU and coworkers, and the subsequent implementations in massively parallel codes have similarly shed much light on the properties of correlated electronic materials. Massively parallel molecular dynamics codes like NAMD or LAMMPS have had a direct role in advancing the study of biomolecular materials. Through this RII, the engine of scientific discovery that drives the development of formalisms, algorithms, and codes in one area will also drive tremendous advances in other areas because the Science Drivers are tightly integrated by the common set of challenges. Thus, the strategy to ensure the largest impact is to develop collaborations between groups representing the research areas in computational materials science that are consistent with the jurisdiction's long-term S&T strategic plan. The emergence of a new paradigm in high-performance computing, i.e., the inevitable shift from multiprocessor machines to multicore and heterogeneous architectures, provides LA-SiGMA with exciting opportunities and challenges for truly transformative developments.

The research program of LA-SiGMA will be structured around three Science Driver teams of experimentalists, theorists, and computational scientists and one Computational team. For the greatest impact, the majority of Alliance researchers will be members of one or more Science Driver teams as well as the Computational team. The latter team will develop formalisms for multiscale materials simulations relevant to all three Science Drivers. The Computational team will also include experts 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 teams will use these tools for generating testable predictions for systems of great technological and scientific interest. These predictions will be validated by experimentalists on the Science Driver teams, making use of existing materials research facilities in the State. 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.

The Alliance members are: Louisiana State University (LSU, lead institution), Grambling State University (Grambling), Louisiana Tech University (LA Tech), University of New Orleans (UNO), Southern University at Baton Rouge (SUBR), Tulane University (Tulane), and Xavier University (Xavier). Grambling, SUBR, and Xavier are classified among "Historically Black Colleges and Universities" (HBCUs).

Strategic Fidelity. The goal of simulation-guided studies of materials is well aligned with the State's master plan for economic development and statewide computational, experimental, and intellectual assets. These assets include the Louisiana Optical Network Initiative (LONI), *the most advanced* high-performance computing (> 80 TFLOPS) network (40 Gbps) and communication infrastructure among EPSCoR states. LONI will devote at least 10% of its computational resources to the project. LONI and the LONI Institute were established through significant State investments; the Institute allows the recruitment of talented faculty to Louisiana. These investments form the nucleus of our Alliance. These efforts are in accord with *Louisiana: Vision 2020*, the master plan for Louisiana economic development, which targets information technology, materials, and biotechnology. The Alliance will leverage existing investments in experimental materials science facilities, including the Center for Advanced Microstructures and Devices (CAMD, the State's own synchrotron source), the Institute for Micromanufacturing (IfM), the Advanced Materials Research Institute (AMRI), and the Center for BioModular Multiscale Systems (CBM^2). The current NSF RII award to develop statewide cybertools and previous awards to the jurisdiction have established the infrastructure needed to support the current proposal as well as the collaborative framework for ensuring its success. All elements of the external engagement and workforce development plans are focused on the development of sustained excellence in computational materials research. To this end, the State pledges $2M cash match per year for the five-year duration of this RII project.

Broader Impacts and Value Added. The project will impact education and workforce development in the State by creating a comprehensive set of programs addressing various demographic needs. These efforts will result in major transformations in education, research, and workforce development in the State, as follows.

Education and Human Resource Development: Pipelines to advanced education will be created through

joint programs such as the 4+1 program between Grambling and LA Tech for undergraduates to gain an Applied Physics MS degree in five years of study, the 3+2 dual degree program between Xavier and Tulane, and the 2+2 program between SUBR and Baton Rouge Community College. We will also leverage a new interinstitutional PhD program in Materials Science (collaboration between LSU, SUBR, and UNO) and an interdisciplinary PhD in Molecular Sciences and Nanotechnology at LA Tech that will be proposed to the Louisiana Board of Regents. Tulane is recruiting an endowed chair in materials science for their newly created Division of Physical and Materials Science. We will provide specialized interinstitutional courses for graduate and postgraduate students who will enter the workforce as highly-skilled, well-trained computational materials scientists. These courses will be integrated into the curricula of the PhD programs to ensure their sustainability. The graduate education program will be unique in the statewide delivery of new courses to support the degree programs mentioned above, using synchronous HD video as well as asynchronous methods.

Diversity: Under the guidance of LA-SiGMA's Diversity Advisory Council, specific recruiting and retention measures are planned to increase the participation of women and underrepresented groups in the activities of the Alliance, including summer fellowships for undergraduates and research supplements of up to $15,000 for graduate students. Project funds will be used to help recruit outstanding women/minority faculty into Alliance institutions. The Louis Stokes Louisiana Alliance for Minority Participation (LS-LAMP), Louisiana's implementation of NSF's Bridge to Doctorate program, will also be leveraged for this project. Our goal is to double the women/minority membership in the Alliance by the end of the project period.

Workforce Development: A comprehensive workforce development plan is proposed, which includes programs designed to involve high school, two-year college, and undergraduate students in research. Our Research Experience for Teachers (RET) programs will train high school and two-year college instructors in inquiry-based teaching methods focusing on computational materials science. Short courses will be offered to two-year college students to train them in the use of state-of-the-art laboratory instrumentation as well as current and next generation high-performance computing systems. Internships and extended visits to industries, national laboratories, and international research centers will broaden the training and career options of graduate students and postdocs.

External Engagement: Through Louisiana Public Broadcasting programs, web portals, newsletters, press releases, and public lectures, we will inform and engage the general public in our pursuit of this transformative research and educational initiative. Outreach to the worldwide scientific community will be accomplished through websites for distributing codes and technical knowledge developed within the Alliance. The Alliance will use existing industrial liaisons to communicate research progress to industries that may have a strong interest in our discoveries. Extensive use of cyberinfrastructure will enhance internal communications as well as interactions with external stakeholders, including the NSF.

Evaluation and Assessment: Rigorous evaluation and assessment by an external evaluator and oversight by an external review board will ensure that project goals and objectives are met. Board members will come from diverse backgrounds and specialties. A comprehensive evaluation plan is based on milestones for research, diversity, workforce development, external engagement, and sustainability.

Sustainability: By leveraging prior NSF EPSCoR investments and state-funded research facilities, we will build statewide interdisciplinary research collaborations involving computational scientists, computer scientists and engineers, applied mathematicians, theorists, and experimentalists. We will build a sustainable interinstitutional computational materials science graduate program. Thus, LA-SiGMA will bring about a transformative and sustainable impact in computational materials research, education, and applications throughout Louisiana, and position the State to compete for and secure the first federally funded center of excellence for simulation-guided materials applications in Louisiana.

The proposed initiatives will be sustained through a variety of mechanisms. Curricular reforms will be institutionalized through new PhD programs. The center of excellence will fund continuing external engagement and workforce development activities. Aggressive recruiting of faculty and graduate students will increase the diversity and competitiveness of the research and education enterprise. Seed-funding programs and statewide workshops and conferences supported by the LA EPSCoR office will further contribute to the sustainability of LA-SiGMA initiatives and build research capacity in the State.

4.1 Status and Overview

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 Louisiana. We will accomplish this by leveraging existing statewide computational, experimental, and intellectual assets.

Modern materials that drive today's technology exhibit "complex emergent phenomena," which refers to properties that emerge from the collective behavior of the fundamental building blocks. Such properties are qualitatively different from the behavior of the constituent atoms and molecules. The principal barrier in the simulation-guided journey from molecules to materials is this emergence of collective phenomena that span multiple length and time scales. A recent Department of Energy Basic Energy Sciences Advisory Committee (BESAC) report[1] cites the "*inability of existing experimental and theoretical techniques to deal with the real-world nanomorphologies*" as an obstacle to first-principles design of new industrial catalysts. Another report on grand challenges[2] devotes an entire chapter to "Emergence of Collective Phenomena: Strongly Correlated Multiparticle Systems." Due to their collective nature, these phenomena elude reductionist approaches. For example, the properties of a helium atom give no hint of the superfluidity of liquid helium, but such properties are clearly ingredients of quantitative treatments that include the large length scales that do reveal superfluidity. Other examples include the dynamics of the Earth's molten core,[3] and the dynamics of our Sun.[4] NSF, on the first page of its report,[5] "*Cyberinfrastructure Vision for 21st Century Discovery*," identifies similar problems, including weather modeling and protein folding, as only now being answered, and then goes on to say, *"Coupled with continuing improvements in microprocessor speeds, converging advances in networking, software, visualization, data systems and collaboration platforms are changing the way research and education are accomplished.*" Treatment of multiscale challenges that cross the boundaries between conventional disciplines requires teams of researchers with expertise at each scale. New algorithmic and computational methods, and teams that incorporate applied mathematicians and computer scientists must be assembled to confront this challenge. In addition, close collaborations with experimentalists are needed to validate the computational predictions. Addressing this need *requires peer-to-peer collaboration that spans multiple disciplines, new modes of research and education, and virtual organizations that work across institutional boundaries*.

LA-SiGMA will address this need by creating a statewide research and education program focusing on (1) electronic materials, (2) energy materials, and (3) 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 forty 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. 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.

Strategic Fidelity and Impact of this project are enhanced by Louisiana's investments over the past two decades in computational, experimental, and intellectual assets that make the jurisdiction well prepared to achieve these objectives. The components that make this plan most compelling and timely for Louisiana (Fig. 1) are the Louisiana Optical Network Initiative (LONI), *the most comprehensive and robust* CI among EPSCoR states; leveraging the current RII cybertools project; a confluence of internationally-known materials science r*esearchers;* and long-standing and successful *experimental facilities* for materials research. In the next few paragraphs, we outline the *strengths, barriers, and opportunities for development of Louisiana's Research and Development enterprise*.

Strengths. Louisiana hosts a diverse and geographically distributed group of 21 four-year public and private universities that serves a population of 4.5 million. There are five PhD-granting institutions, two of which (LSU and Tulane) are Carnegie Research University/Very High. The State has several minority-serving institutions. Xavier University, according to the U.S. Department of Education, ranks first nationally in the number of African American students earning undergraduate degrees in both the biological/life and the physical sciences. The Southern University (SU) system is the only historically black university system in America with an enrollment of over 15,000 students, offering 86 baccalaureate, 23 associate, 26 master's, and 5 doctoral degree programs.

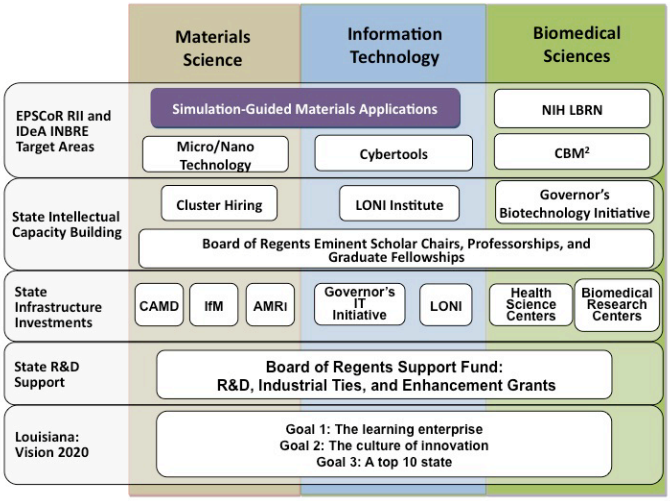


Fig. 1. Louisiana's targeted investment strategy. (Acronyms are expanded in the text.)

Following *Louisiana: Vision 2020* – the master plan for economic development – the current and past two gubernatorial administrations have strategically supported Louisiana's R&D enterprise. Vision 2020 targets specific Science and Technology (S&T) areas for investment: Information Technology, Materials, and Biotechnology. In 2002, the Governor's Biotechnology Initiative provided $2.75M in annually recurring funds and $5.7M in one-time funds to enhance state-of-the-art biotechnology research. Louisiana's Information Technology Initiative invests $25M annually, including $9M annually for the LSU Center for Computation and Technology, to develop S&T faculty expertise. This initiative recruits top-notch faculty, strengthens the State's IT infrastructure, and enables the creation of new academic programs to enhance the workforce required by current and new IT-intensive businesses in Louisiana.

In 2004, the State further committed $4M annually over 10 years to build its research CI via LONI. This world-class tool offers Louisiana research opportunities and a gateway to the world. Louisiana has received national accolades for its vision and commitment to sustainability in deploying this groundbreaking network. In 2006, an additional $10M was invested in High-Performance Computers (HPCs) including a 50-TFLOP computer that ranked 5th among academic institutions worldwide when introduced in 2007. The total computing capacity of LONI is 85 TFLOPS. With these resources, Louisiana was chosen as one of a small number of NSF TeraGrid resource providers.

Strengths: Physical Infrastructure for Experimental Materials Science. The project will leverage shared experimental resources. The *Institute for Micromanufacturing* (IfM) facilities at Louisiana Tech University (LA Tech) will be used to study hydrogen absorption/desorption, catalytic conversion of biomass to biofuels, and the use of clay nanotubes for controlled release of drugs. Researchers at the *Advanced Materials Research Institute* (AMRI) at the University of New Orleans (UNO) will perform measurements on nanoscale magnetic and ferroelectric materials and novel electrochemical devices based on nanotube forests. The synchrotron at the *Center for Advanced Microstructures and Devices* (CAMD) at LSU will be used to

study hydrogen storage and retrieval and strongly correlated electronic systems. The *Center for BioModular Multiscale Systems* (CBM^2) at LSU will synthesize, characterize, and study the encapsulation and transport properties of biomolecules.

Strengths: Physical and Intellectual Infrastructure for Computational Research. In addition to LONI, LSU's Center for Computation and Technology (CCT) provides additional resources for this project. CCT scientists will adapt and extend the "CyberTools" developed during the current RII project to the needs of this project, including data archiving, retrieval, reuse, and visual data analysis. CCT will guide the acquisition of and training on the next generation CI.

Strengths: Intellectual Infrastructure for Materials Research. The State's LONI Institute (institute.loni.org) is a recent joint collaboration between six research institutions, created by a $15M investment by the State, through which faculty are being hired in targeted areas of materials and computational science. The Institute is a virtual organization in which hiring and strategic planning decisions are shared between the six institutions. Other hiring initiatives have led, for example, to LSU's recruitment of its first National Academy of Sciences member (Ward Plummer) and five additional materials science faculty.

Barriers. The relatively large number of research institutions and resulting lack of a critical mass of intellectual capital at a single location is a major barrier to achieving national competitiveness in Louisiana. Cooperative research among institutions is thus the best strategy to attaining national competitiveness in this relatively poor state. By funding large-scale, multidisciplinary projects with intra- and inter-institutional collaborations that leverage resource sharing, EPSCoR has had a transformative impact on the State. This momentum must continue for Louisiana to become nationally competitive. Through previous initiatives, Louisiana has begun to attract top-notch faculty and researchers to the State. What remains is to focus the investment and resources on targeted research areas of national need to propel the State to the next level of competitiveness. LA EPSCoR, in partnering with the State, aims to accomplish this goal through this RII proposal.

Opportunities. LA-SiGMA will address these barriers by forming a highly focused statewide research consortium which capitalizes on intellectual talent, combines the pertinent elements developed under previous RII awards, and leverages the state-of-the-art CI that has recently become available to position Louisiana as a major hub of innovation in computational materials science. LA-SiGMA features comprehensive plans for education, external engagement, and workforce development. Although focused in terms of research areas, the Alliance is truly a statewide effort involving seven campuses and roughly 54 investigators who will be members of interdisciplinary and interinstitutional teams. This critical mass of investigators is a significant strength of this proposal and is made possible using shared graduate students that increase the number of faculty participants and a stringent assessment structure that will ensure all participants are working in a coordinated and effective manner. The sustainability plan is designed to position LA-SiGMA to compete for a federally funded center of excellence in simulation-guided materials applications by the end of the five-year project. The intellectual capital and long-term interinstitutional collaborations further generated by this RII project will lay the foundations for this effort.

The Louisiana Board of Regents (BoR), the statewide agency that coordinates State universities and colleges, will make significant contributions to the project. The State will contribute $2M cash match per year for the five-year duration of this RII project. Louisiana EPSCoR, which is housed at the Regents, is crucial to BoR's arsenal of initiatives aimed at advancing the State's research infrastructure. By Executive Order, the Governor recently established the Louisiana Innovation Council that will "develop and implement targeted policies, programs, and investments designed to maximize the potential of our increasingly knowledge-based economy." The Governor's staff charged the Regents and EPSCoR leadership to assist in framing the work of the Council for advancing Louisiana's R&D enterprise and its impact on the future economic competitiveness of the State. Specifically, Michael Khonsari, the PI of this proposal and EPSCoR Project Director, has been appointed by the Governor to serve on the Louisiana Innovation Council.

The **payoff** from this project will be significant. LA-SiGMA will transform research and education in computational materials science throughout Louisiana. The Alliance will have more than 100 faculty, postdocs, and students and will be sustained by collaborations involving shared students and postdocs, new PhD programs in computational materials, new courses taught via synchronous HD video, and aggressive pursuit of external funding that will lead to a national center of excellence.

4.2 Results from Relevant Prior NSF Support in the Last Five Years

EPS 0346411: (2004-2007) Louisiana's Strategic Infrastructure Improvement (PI: Michael Khonsari): This RII award initiated the Center for BioModular Multi-Scale Systems (CBM^2) involving multidisciplinary teams of science and engineering faculty from LSU, CAMD, LSU Health Sciences Center - New Orleans, Tulane Health Sciences Center, and Xavier. Over the grant period, CBM^2 researchers prepared a total of 384 scientific publications, gave 304 presentations, and secured $10M in external funding. CBM^2 has developed new chemistries and materials (molecular, nanometer, and micron scale) that can be integrated into high-performance devices spanning several size scales, increasing their functionality and cost-effectiveness through integration, and accelerating advancements in basic biological sciences and forensics. In addition, a statewide S&T seed funding program (Pfund) was initiated. Funding in the amount of $400K resulted in $15M in external funding and 71 publications. **Relevance to proposed activities**: In the proposed project, CBM^2 researchers will synthesize, characterize, and study the encapsulation and transport properties of biomolecules. The Pfund program was successful in catalyzing research in emerging areas; therefore it is included as an element of the subsequent RII, as well as the proposed project.

EPS 0701491: (2007-2010) Louisiana's Research Infrastructure Improvement Strategy (PI: Michael Khonsari): This current RII grant features the development of CI tools, or "CyberTools," with four Work Packages designed to facilitate development of (1) scheduling and data services; (2) information services and portals; (3) visualization services; and (4) application services, toolkits, and algorithms. These tools are being developed in concert with innovative research in biosensor development and biotransport processes. As of June 2009, outcomes include over $17M in external funding, with $75M pending, 144 publications, and two patents awarded. **Relevance to proposed activities**: This project has demonstrated the potential transformational impacts of computational science tools (CyberTools) to the advancement of science in the physical domain. It began to bring computer scientists together with domain scientists in the solution of complex problems. The CyberTools developed under this award will be adapted and extended to the needs of this project, including data archiving, retrieval, reuse, and visual data analysis.

OCI 0710874: (2007-2009) HPCOPS: The LONI Grid - Leveraging HPC Resources of the Louisiana Optical Network Initiative for Science and Engineering Research and Education (H. Liu (PI), S. Jha (co-PI)): Through this project, Louisiana provides 50% of "Queen Bee," a 50 TFLOP, 5,028 core Dell Linux cluster that employs Intel's multicore processor technology, to the NSF TeraGrid. LONI is one of only 11 TeraGrid sites. **Relevance to proposed activities**: This award brings improved access to the TeraGrid for Louisiana researchers, and through associated training, prepares researchers for using NSF's current and future leadership class of supercomputers.

HRD 0503362: (2005-2010) Phase III - Louis Stokes Louisiana Alliance for Minority Participation (LS-LAMP) (PI: Diola Bagayoko): LS-LAMP is a statewide mentoring program to increase the number and quality of minority students earning baccalaureate degrees in STEM disciplines and to actively promote their transition to STEM graduate schools for the pursuit of terminal (PhD) degrees. The Phase III award seeks to (1) consolidate and augment the achievements of Phases I and II; and (2) maximize the transition of minorities holding BS degrees in STEM disciplines to graduate STEM programs and research careers. **Relevance to proposed activities**: Dr. Bagayoko, who is also a member of the LA-SiGMA project execution team (see 4.10), will provide his expertise to create a supportive environment for Underrepresented Minorities (URM) in STEM disciplines.

4.3 Research Program

The study of collective emergent phenomena through the development of experimentally validated multiscale computational models provides significant opportunities for transformative materials research. A schematic representation of the general plan for the proposed research program is provided in the **Project Summary**. A major research focus of the Alliance will be to develop and experimentally validate common computational tools essential for three Science Driver (SD) areas of current strength in the State, and of great technological and economic importance: **(1) electronic materials, (2) energy materials, and (3) biomolecular materials**. The Alliance has roughly equal numbers of computational scientists/theorists and experimentalists and the proposed research budget is allocated accordingly. The research activities of the Alliance will be organized through three SD teams and one computational team. Alliance computational scientists will be members of at least one SD team as well as the computational team. The SD

teams will develop new formalisms and methods for tackling multiple length and time scales and multiscale interactions and correlations. The computational team will include experts who will help translate these formalisms and methods into algorithms and codes that take advantage of current and anticipated high-performance computing platforms. The commonality of the tools will be a major factor that tightly integrates the three Science Drivers. The SD teams will use these tools for generating testable predictions for systems of great technological and scientific interest. These predictions will be validated by experimentalists on the SD teams, making use of existing materials research facilities in the State. A feedback loop will develop between the experimentalists and the other team members to refine the formalisms, while also enhancing the collaborations between experimentalists, theorists, and computational scientists. Students and postdocs will work in a multidisciplinary team environment, providing a unique experience that enhances the training and educational impact of this project. The overlapping memberships of teams will ensure that advances in one area are rapidly communicated to other areas. Ultimately, the experimentally validated computational approaches will position LA-SiGMA and the State to advance simulation-guided materials science and position the State to compete effectively for a federally funded center of excellence in simulation-guided materials applications.

In the following sections, we describe the common computational tools and the proposed efforts in the three SD areas; also described is the coordination plan. *The lead investigators for each effort are shown in brackets*.

4.3.1 Common Computational Tools for Multiscale Simulations

The "glue" that holds the three SDs together (Fig. 2) are the formalisms, algorithms, and codes to be developed during the course of this project. Therefore, to achieve the goals of this RII project, we have assembled a **cybertools and cyberinfrastructure (CTCI) group** of 27 participants, led by Jha (LSU), that will allow Alliance members to more efficiently utilize the next generation of 21st-century supercomputers, including Blue Waters.[6] The CTCI group will have four focus areas: (i) Novel Architectures [Ramanujan (LSU)], (ii) Execution Management Tools and Environment [Allen (LSU)], (iii) Visualization [Jana (SU)] and, (iv) Distributed Data Management and Provisioning [Kosar (LSU)]. The present state-of-the-art petaflop computers have tens of thousands of processors. Alliance members have extensive experience with these machines and have achieved efficient scaling to 10,000 processors. The next generation of hyperparallel, heterogeneous, and multicore machines will present additional challenges that can only be overcome with the shared experiences of the CTCI teams and applied mathematicians [Lipton and Bourdin (LSU), Dai (LA Tech)], and Li (SU) and experts in high-performance computing [Jha, Sterling, Ramanujam (LSU) and Leangsuksun (LA Tech)]. The CTCI group will build upon the current RII-Cybertools project to provide the end-to-end computational tools, environments and capabilities to enhance the utilization and productivity of high-performance and distributed CI. This will enable the Alliance computational capabilities to both Scale-Up and Scale-Out, a balance of which is required to effectively utilize both the next generation of high-end machines (e.g., Blue Waters), as well as prepare the Alliance for the next phase of distributed national CI, namely, the TeraGrid XD (mid-2011). The Alliance will build transformational common toolkits around three core formalisms/algorithms indispensable for computational materials science, as outlined below.

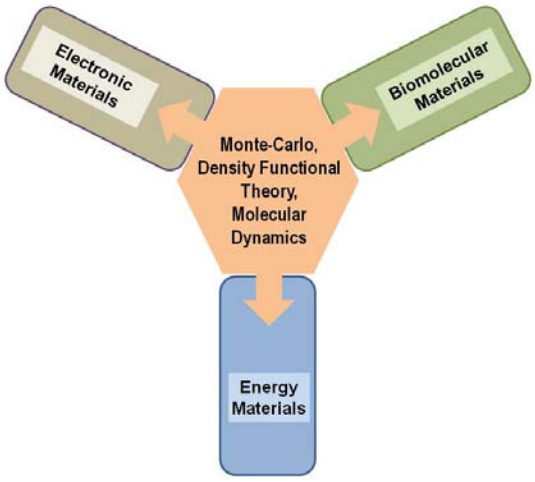


Fig. 2. Science Drivers are linked by common computational tools.

Next Generation Monte Carlo Codes [Pratt (Tulane), Jarrell (LSU), Mobley (UNO)]. Monte Carlo (MC) simulations can bypass long time scales by directly calculating free energies associated with activated (long time) processes and by allowing dynamical properties to be studied without following the dynamics serially.[7,8] MC methods are employed in studies of phase equilibria, nucleation, protein folding, and electronic structure and will be used in all three SD teams. They allow simulations to be split into independent processes representing, for instance, different realizations of quantum state behavior, different parameters (such as temperature), or simply by subdividing the MC Markov process. Therefore, many MC codes

are inherently parallelizable. However, these codes will not be efficient on the next generation of multi-core, hyperparallel, or heterogeneous machines being developed as part of the 21st-century CI.[5] Many of these problems can be resolved through the development of hybrid-parallel codes. The MC team will work closely with experts like Ramanujan (CTCI group) to develop a suite of next generation MC codes that will be used by all the SD teams.

Massively Parallel Density Functional Theory and Force Field Methods [Perdew (Tulane), Wick (LA Tech), Bagayoko (SU)]. Density Functional Theory (DFT) with Generalized Gradient Approximation (GGA)[9] has allowed computational chemistry to become an indispensable tool in all branches of molecular sciences. One of the most successful and systematic approaches to developing density functionals with broad applicability was pioneered by Perdew at Tulane,[10] who will lead the development of more accurate GGA functionals. The most recent functional from the Perdew group, the revTPSS-2009,[11] holds great promise as the starting point for a fully nonlocal functional needed to describe correlated systems such as transition metal oxides. Such a functional will find immediate application in two SDs, namely, electronic and energy materials. We will also examine the M06 family of functionals from the Truhlar group[12] that can describe long-range and non-bonded interactions that are important in biomaterials. The force field team led by Wick will design reactive and transferable (to different state points, mixtures, and interfaces) force fields for improved predictive ability. The computational team will help implement the new DFT functionals and force fields on multicore and heterogeneous platforms to allow SD teams to perform large-scale computations. These high-performance codes will be central to advancing all three SDs. The execution management team (Allen) of the CTCI group will work closely with Perdew, Bagayoko and Wick, to enable complex workflows, ensemble runs, and multiple-stage calculations to exploit the full potential of novel machines like Blue Waters.

Large-scale Molecular Dynamics [Ashbaugh (Tulane), Jha (LSU), Rick (UNO)]. While MC simulations can study the statistical properties of long time scale processes, simulating the dynamics at the molecular level requires Molecular Dynamics (MD) methods. Following the dynamics of multiple length scales (molecular to mesoscopic) demands a sophisticated and consistent treatment of the different length scales. Therefore, reliable MD simulations are critical for multiscale materials simulations. NAMD, Gromacs, and LAMMPS (http://lammps.sandia.gov/), are open source classical MD codes used for modeling atomic, polymeric, biological, metallic, granular, and coarse-grained systems. New algorithms and codes based on a variational approach and hybrid MD/continuum methodologies will be developed and added as modules to the LAMMPS package. We will work in partnership (see letter of commitment) with Sandia National Laboratories, the distributor for LAMMPS, which is designed for parallel computers that support C++ compilers and MPI message-passing library. The CTCI team will work with the SD teams to port LAMMPS to the next generation supercomputers in which MPI may not be the optimum solution. They will also lead the efforts to incorporate new (Sec. 4.3.2, Science Driver 2) or existing (such as ReaxFF[13]) force fields into the LAMMPS program. The visualization team (Jana) of the CTCI group will work with the MD team to develop the space-time multiresolution visualization capabilities as well as integrate them within existing immersive and interactive environments.

4.3.2 Science Drivers (SDs)

SD1: Electronic and Magnetic Materials [M. Jarrell (LSU), J. Perdew (Tulane)]

Many electronic and magnetic materials are characterized by strong correlations. They are the paradigm for complex emergent phenomena involving the many *length* scales **barrier**, as these materials exhibit long-ranged order (on the scale of the sample size) that emerges from atomic spin, orbital, and charge degrees of freedom (on the scale of 10^{-10} cm). The current **state of the art** uses spatially local approximations like Local Density Approximation (LDA) and the Dynamical Mean Field Approximation (DMFA).[14,15] The **goal of this SD** is to transform the field by extending these methods to much larger length scales. The development of multiscale methods for strongly correlated electronic and magnetic systems is **novel**, and will involve a team of 26 faculty that includes experts in relevant computational and DFT methods and an experimental team that includes experts in a wide variety of measurement techniques. The **payoff** of this collaboration will be the ability to accurately model strongly correlated materials on national leadership supercomputers for the first time.

Strongly correlated materials have many promising applications. The 2007 International Technology Roadmap for Semiconductors[16] stresses that highly correlated electron systems can enable new devices

by greatly enhancing their sensitivity to different applied fields. Organic magnets are highly tunable systems that will lead to a better understanding, which will help with the design of higher-performance magnets, e.g., with higher blocking temperatures. Several studies have been performed on molecular magnets as potential labeling and imaging agents for biology and medicine.[17,18] Organic semiconductors are tunable, flexible, easier and cheaper to fabricate, and have long spin coherence lifetimes.[19,20] In each case, it is the complexity of these materials that makes them promising, i.e., the ability to use the competing spin, charge, or orbital ordering to gain sensitivity to various fields, or the use of both the spin and charge degrees of freedom in spintronic organic semiconducting devices.

Strong correlations can lead to emergent phenomena, including spin, charge, and orbital ordering. The complexity is further enhanced by a competition between states that is displayed by many strongly correlated materials, including heavy Fermion materials, transition metal oxides, high-temperature superconductors, spintronic materials, manganites, and organic magnets and semiconductors. These technologically promising materials are poorly understood due to long-ranged spin and charge correlations, competing ground states, and their complex phase diagrams.[21] These competing states have both local (e.g., commensurate magnetism) and highly nonlocal (e.g., charge ordering) order parameters. ***Multiscale approaches*** are essential to treat both the development of long-range order *and* the competition between these states.

SD1, Focus 1: Multiscale Methods for Strongly Correlated Materials. Investigators using the present set of numerical methods have begun to understand the individual phases of these systems. DFT, notably the Local Density Approximation (LDA), accurately describes a host of moderately correlated materials. A variety of augmentations ("LDA+" methods) allow DFT to address the role of stronger local correlations. A notable example is the combination of LDA or down folding LDA calculations[22,23] with the Dynamical Mean Field Approximation (DMFA)[14,15] and its cluster extensions, including the Dynamical Cluster Approximation (DCA).[24-27] These methods have, for example, provided a qualitative understanding of the origins of antiferromagnetism and superconductivity in some systems. Yet these algorithms are fundamentally limited in their treatment of the different length scales. To understand the complexity that emerges due to the competition between different phases, a new suite of computational formalisms, algorithms, and codes is required. The SD team will attack the *grand challenge problem of multiscale physics in strongly correlated systems* by developing and applying **novel** methods that systematically incorporate nonlocal corrections to both LDA and DMFA.

The ***barriers*** that inhibit these developments are inherent to existing computational methods. DMFA[14,15] and DCA[24-27] map the lattice onto a cluster embedded in a self-consistently calculated effective medium. The cluster problem is usually solved using a Quantum Monte Carlo (QMC)[28-30] simulation, while disorder can be included by averaging over configurations.[24-26] Currently, either perfectly parallel (MPI) or hybrid parallel (MPI+OpenMP) calculations are used. For this project, in conjunction with the CTCI Novel Architectures team (Ramanujam), we will develop a hybrid continuous time QMC solver for 16-way multicore, hyperparallel computers such as NSF's Blue Waters. Nevertheless, calculations are limited by the "minus sign" problem, which is nonpolynomial hard.[31] This means that simulations of correlated electrons take exponentially longer as temperature decreases and cluster size increases, making it very difficult to treat correlations on the important length scales. Another issue is that the LDA is an approximation based upon the numerical solution of the Homogeneous Electron Gas (HEG). Since the HEG does not have ordering or moment formation, it is difficult to describe these phenomena using LDA.

Significant developments beyond the state of the art are required to ***address these problems***. For example, in the DMFA/DCA approach, another length scale must be introduced as in the Multiscale Many Body (MSMB) approach.[23,32] This is accomplished by a multiple embedding scheme in which correlations over each length scale are treated with an appropriate approximation. Strong correlations at short length scales are treated with a numerically exact QMC simulation on a small cluster. This cluster is embedded in the larger cluster where the weaker correlations at intermediate length scales are treated using the parquet approximation.[33-37] This larger cluster is embedded in an effective medium that is used to treat correlations on the longest length scales. For this project, we will develop an MSMB code capable of treating multiple correlated orbitals. For DFT, the Perdew group will develop a complementary approach to the strongly correlated electron problem that relies upon improved approximations for the exchange-correlation energy. A recent meta-GGA[11] , which predicts accurate lattice constants and surface energies for solids and accurate atomization energies for molecules, is probably close to the limit of accuracy for

semilocal functionals, and is a natural base on which to build the fully nonlocal approximations. A hyper-GGA currently under development[11,38] based on these ideas, describes the strong correlation responsible for high energy barriers to chemical reactions, and also the moderate correlation present in ordinary matter. This functional will be incorporated into common DFT codes including VASP.

The **payoff** from these developments will be the greatly improved ability to study the correlated systems described in Foci 2 and 3, where overcoming the multiscale barriers will be transformative.

SD1, Focus 2: Correlated Organic and Ferroelectric Materials. Studies of organometallic conductors and magnets will be performed using porphyrins and iron oxide clusters coated with biocompatible small-molecule capping ligands as testbeds. Porphyrins are excellent model systems for fundamental studies of the interrelationships between electronic properties and structure, due to their robust and versatile structural motifs, which allow production of a rich variety of molecular architectures.[39-43] Molecular clusters formed by high-spin mid-3*d*-transition metals exhibit different forms of magnetic behavior, including ferromagnetism with slow relaxation rates.[44-47]

Perdew, Ruzsinszky, and Burin (Tulane) and Derosa (LA Tech/Grambling) will study metalloporphyrin nanostructures to test and validate a wide range of DFT functionals, including the Local Spin Density Approximation (LSDA), the second generation GGA functionals, and the more recent meta- and hyper-GGA functionals developed by the Perdew group. Jarrell and Moreno (LSU) and Fishman (Oak Ridge National Labs) will use the calculated band structures to construct Hamiltonians that will be used in a DMFA/DCA study of the dynamic magnetic properties. These same Hamiltonian parameters will be used by Browne (LSU) and Derosa in nonequilibrium Green function calculations[48-51] of charge transport in these systems. Garno[52,53] (LSU) will prepare nanostructures of metalloporphyrins and perform magnetoresistance and electrical conductance measurements for comparison with and validation of the computational methods.

Burin, Ruzsinszky, and Perdew will use the new functionals to study high-spin molecules, such as iron oxide clusters (Fig. 3) embedded in organic molecules. To validate the computational approaches, Spinu (UNO) joined by Stevens and Goloverda (Xavier) will measure cluster magnetic properties using Squid Magnetometry[54,55] techniques at UNO/AMRI with samples synthesized by Kolesnichenko[56,57] (Xavier).

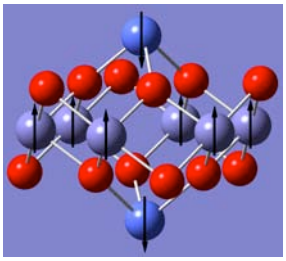


Fig. 3. Iron oxide clusters used as organic magnets will be characterized by electronic and vibrational structure, spin-ordering, and magnetic states and anisotropy barrier [*Ab initio* calculations by Kolesnichenko (Xavier)].

The complex emergent phenomena of multiferroic composites allow the interconversion of electric and magnetic energy.[58,59] This is an emerging class of multifunctional materials for smart sensors, computer memories (utilizing both charge and spin to store and process information), and voltage-controlled magnetic devices such as tunable microwave filters.[60-62] Malkinski and Caruntu (UNO/AMRI) and Meda (Xavier) will fabricate nanostructured multiferroic composites, and Whittenburg (UNO) will perform computer simulations using Perdew's GGA methods to predict the magnetic, ferroelectric, mechanical, magnetostrictive and electrostrictive properties and model devices constructed using these materials.

SD1, Focus 3: Superconducting Materials. These methods will also be used to study the new pnictide[63,64] and cuprate superconductors. The pairing mechanism in the pnictide materials has not been established. Proposals include phonons, correlation effects enhanced by nesting,[65] or a more novel mechanism involving overscreening of the Fe-Fe interaction by As.[66] Methods that combine LDA and MSMB/DCA will be used by Browne, Moreno, Vekhter, and Jarrell (LSU) and Bagayoko (SU) to study the first two mechanisms. Assessing the overscreening mechanism requires Perdew's new DFT methods, since conventional LDA will not capture the nonlocal effect of an As atom screening the interaction between adjacent Fe atoms, a major feature of the third mechanism. A central question surrounding the cuprates is: "What is under the superconducting dome?"[67] surrounding a Quantum Critical Point (QCP) that was recently found in model calculations.[68] The question of whether the order associated with the QCP, if any, competes with superconductivity must also be addressed. A new generation of massively parallel QMC and MSMB codes will be used to address these questions. For example, bottlenecks in the parquet equations include the contractions and rotations of large (greater than 100GB) rank three tensors (vertices), as well as numerical instabilities, which can be addressed with massively parallel linear sys-

tems solvers, such as BICG, BICGStab, or GMRES. These new codes will be developed by an extensive collaboration involving researchers at the Center for Computation and Technolgy CCT, including Ramanujam (the developer of advanced tensor rotation and contraction methods), Jarrell, and Moreno (LSU), together with Tomko (Ohio Supercomputer Center), Fishman (Oak Ridge National Laboratory), as well as the computational team. This team will focus on the calculation of thermodynamic and transport properties, which will be validated by Diebold and Mao (Tulane); and neutron and ARPES spectra, which will be validated by Plummer and DiTusa (LSU) and Sprunger and Kurtz (CAMD/LSU); all using samples made by Jin and Zhang at LSU (see letters of commitment).

SD 2: Materials for Energy Storage and Generation [L. Pratt (Tulane), C. Wick (LA Tech)]

Efficient and clean generation and use of energy are major challenges facing the nation and the world. Alliance members will study electrochemical cells and capacitors that store and deliver electrical energy, advanced materials for the storage and release of hydrogen, and catalytic reactions that generate hydrogen gas. These inquiries are tightly bound by the common **barrier** of multiple scales. For example, significant energy storage involves the short length scales of molecular chemistry, efficient delivery involves energy and material transport over longer length scales, and the microstructure provides material design variables. The essential length scales range from 10^{-10} m to 10^{-3} m, and essential time scales range from 10^{-12} s to 10^{3} s. In addition to the wide range of length and time scales, other **barriers** include accurate treatment of intermolecular forces using either Quantum Mechanics (QM) or force fields. Quantum simulation is **presently** limited to time scales of ~10^{-11} s, while existing force fields, including coarse-grained versions, are not well tested for the energy applications of interest herein and are limited to time scales much less than one second. The **goal of this SD** is to develop and apply **novel** DFT formulations, reactive and transferable force fields, and high-performance MC/MD methods to address these common challenges. There will be significant overlap in membership between the SD2 team and the CTCI group, as all projects involve DFT, force fields, MC/MD, visualization, and data management. We will combine these methods to treat all relevant scales. A team of 21 faculty with expertise in multiscale simulation methods, DFT, MC methods, and continuum models will perform simulations that will be validated and guided by SD2 experimentalists. The **payoff** from this work will be experimentally validated multiscale *models* that can reliably guide the development of practical solutions to important energy-related problems which, in conjunction with the CTCI group, will utilize dynamic-execution models to reduce the time-to-solution on multiple different architectures (Jha, Allen).

SD2, Focus 1: Electrochemical Capacitors and Fuel Cell Electrodes Based on Nanotube Forests. Fast, high-energy density, electrical energy storage materials will be a disruptive technological advance for effective utilization of intermittent and distributed power sources from the grid, for design of electrical vehicles, and for regenerative energy capture, including automobile braking. Pratt (Tulane) has carried out the first molecular simulations of proposed supercapacitors based on carbon nanotube (CNT) forests (Fig 4).[69] Zhao (SU) has promising preliminary results for the simulation-guided design of CNT-based fuel cell electrode materials. The **goal** of this focus area is to use **novel** MC and *ab initio* methods to overcome the multiple time scales **barrier** and study electrical storage materials. The **payoff** is the ability to design better electrochemical capacitors and fuel cells.

CNT forests are intrinsically multiscale problems. The interactions at the pore surfaces are 10^{-10} m scale and pore radii are ~10^{-9} m scale, while the height of the nanotube forest is 10^{-3} m. A research goal for capacitors is to improve the energy densities while retaining the natural advantages of capacitors of rapid response, long lifetimes, and temperature insensitivity. Molecular-scale simulations of these systems (Fig. 4) are feasible[69] and yield single-electrode capacitances in the neighborhood of 80 F/g of electrode, in agreement with experimental capacitances of electrochemical capacitors utilizing carbon-nanotube forests or carbide-derived carbons as electrode material. The Alliance will extend this work to address a variety of practical issues.

Numerical simulations of pore filling will predict pore composition in important situations where reliable estimates are not available. This will characterize the dynamics over the relevant range of 10^{-9} s to 10^{-3} s for candidate materials. Ashbaugh, Pratt, and Bishop (Tulane) will develop and apply (with CTCI help) MC algorithms applicable to phase equilibria. Current models assume that a quantum capacitance adds in series with the electrochemical capacitance. The Alliance will use DFT methods to test this assumption using atom-level charging of graphite electrodes. Coarse-grained electron density models will be implemented (with CTCI guidance) in large-scale MD simulations. Pesika (Tulane) will carry out cyclic

voltammetry on nanotube forests to explore the potential dependence of the experimental capacitances. The stored energy depends *quadratically* on the electric potential, and operation at potentials as high as 4V could achieve a high energy density. But extraneous chemical damage must be avoided. Incorporation of chemical processes in molecular simulation is at the forefront of materials simulation research. Rick (UNO) will incorporate the reactive impurities from H_2O redox chemistry to simulate damage expected at high potentials.

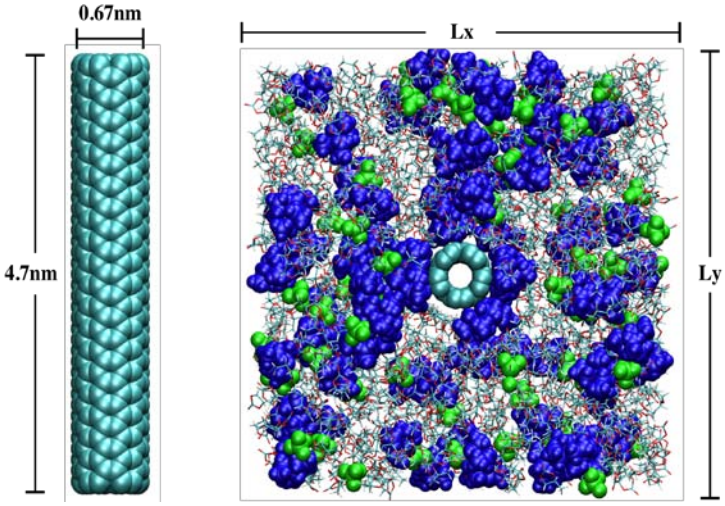


Fig. 4. Design of the molecular simulations. Singe-walled nanotube (left); a simulation cell (right), which is repeated using periodic boundary conditions in all directions. The solvent is propylene carbonate and the electrolyte is tetraethylammonium tetrafluoroborate, routine experimental choices. The calculations utilized AMBER force field models. A realistic surface charge was imposed on the nanotube and the electrostatic potential difference between the conducting solution and nanotube surface was evaluated at equilibrium. Typical simulations treated 1,000 propylene carbonate molecules and 100s of ions for durations of 10 ns [simulations performed by the Pratt group (Tulane)[69]].

Zhao and Bagayoko (SU) will use DFT-MD with Perdew functionals to understand the catalytic mechanism of the oxygen reduction reaction at nitrogen-doped CNTs. Preliminary simulations show that N edge-doped CNTs are the most stable structures. Henry (SU) will build fuel cells with these materials and will evaluate the effectiveness of the new designs. The CTCI group will port these calculations to next generation computers.

SD2, Focus 2: Thermodynamics and Kinetics in H_2 Storage Systems. Among the **barriers** that hinder the use of hydrogen as a clean alternative to hydrocarbon fuels are absorption/desorption rates, volume/weight ratios, hydride stability, and desorption temperatures of current H_2 storage materials. The Alliance will use **novel** multiscale MD and MC simulations, kinetic MC, finite element, and finite difference modeling to predict rates of hydrogen uptake/release over time scales reaching 10^3 s and extending over several microns for metal alloy storage materials with new catalytic additives. Other Alliance members use X-ray tomography to probe these materials over the same length and distance scales. The **goals** of this focus area are to predict the influence of catalytic additives in enhancing atomic mobilities and desorption rates in metal hydrides and to explore a wider range of potential hydrogen storage materials. The **payoff** will be an improved ability to design materials for hydrogen storage.

Ab initio molecular scale energetic, structural, dynamic properties will be calculated by Mainardi (LA Tech). Wick (LA Tech), Chen and Hall (LSU) will develop force fields appropriate for these reactive systems to supplement the ReaxFF force fields. Hall, Chen, Wick, and Mobley (UNO) will use advance ensemble methods[70-80] to calculate the free energies of different compositions and to determine the spinodal points of mixtures. Mainardi and Dai (LA Tech) will study diffusion and reactions using kinetic MC and employ finite element and finite difference methods for extended length and time scales. CTCI group members will port codes, allow data reuse, and provide efficient work flow. Butler (LSU) and Dobbins (LA Tech/Grambling) will employ the LSU X-ray synchrotron tomography beamline and the Argonne Advanced Photon Source nanotomography beamline to study *in situ* and *ex situ* de/rehydrogenation reactions, to assess 3D microstructures and interphase boundaries, and to quantify the distribution and size of single phase domains. The CTCI visualization toolkits will be utilized for this part of the project. Since atomic diffusion rates may limit the desorption, Browne (LSU) will use Fick's Law diffusion and non-equilibrium chemical models to model solid state diffusion and phase transitions.[81-83] The temperature-dependent diffusion coefficients will be determined using diffusion and diffusion-reactions equations and experiments. The results of these simulations, calculations, and experiments will be the prediction of optimum conditions and materials for hydrogen release and uptake.

SD2, Focus 3: Catalytic Reactions Involving Metal Oxides. Metal oxides are an important class of catalytic materials used in industry and are implicated in the formation of hazardous materials when formed in the environment. The scarcity of accurate force fields is the **barrier** that limits modern simulation for these materials. The **goal** of this focus area is to develop **novel,** reliable *and transferable* reactive force fields incorporating polarizabilities and environment dependent atomic charges. The potential parameters will be determined from structural calculations on large systems and charges, and their fluctuation parameters will be calculated from fits to electrostatic potentials. Massively parallel implementations (guided by the CTCI teams) of modern DFT functionals will be used to incorporate the force fields into the calculations of the SD teams. The **payoff** will be the ability to design better metal oxide catalysts and force fields for use in the other SDs.

Burning lignocellulosic biomass (e.g., wood chips) in low oxygen conditions yields water gas, a mixture of CO and H_2O. The water gas shift reaction is used to obtain CO_2 and H_2 from this mixture.[84] The H_2 can then be used as a source of energy. Experimentalists at LA Tech and Grambling have perfected methods for synthesizing metal oxide catalysts that promote this reaction under various conditions.[85] Experimentalists at LA Tech have developed novel nanostructured catalysts that convert water gas to higher hydrocarbons or alcohols using Fischer-Tropsch processes,[86] while avoiding some of the well-known problems with tar formation. Despite their importance, a molecular-level understanding of the catalytic processes in these two reactions is lacking. Complicating their utility, when metal oxide nanoparticles are released into the environment (through, for example, incineration of spent catalysts), they can catalyze production of Polychlorinated Dibenzo-p-Dioxins (PCDDs) and Dibenzofurans (PCDFs).[87] This focus area will study both the beneficial and harmful features of metal oxides.

Rick (UNO), Ramachandran and Wick (LA Tech), and Hall and Chen (LSU) will lead the computational effort using DFT, force field methods, and MC/MD simulations. Siriwardane (LA Tech) and Seetala (Grambling) will synthesize catalysts and use scanning probe microscopy and X-ray diffraction methods to study catalyst structure (see letters of commitment). They will evaluate catalyst performance using flow and batch reactors coupled to gas chromatographs. The computational and experimental team members will work closely, with shared students, to validate the computational models and force fields for metal oxides. Since catalytic processes nearly always involve bond breaking, atomic/molecular migration, and bond formation at different active sites at different times, the ability to deal with multiple length and time scales is essential. The validated models will be used to explore the possibilities of improving catalyst performance, and promising candidates will be examined by Siriwardane and Seetala. These studies will directly benefit two start-up companies in Ruston (Renewable Fuels, LLC, and Carbon Capture Energy Technologies, Inc.) that have provided letters of commitment for this work.

The initial steps in the gas phase formation of PCDDs and PCDFs,[88] and the structure and reactivity of small copper oxide clusters are now being studied[89] to understand this molecular process. Accurate metal oxide force fields and sophisticated MC methods[70-80] are needed to simulate the larger cluster sizes that are being studied experimentally by Dellinger (LSU). Hall and Chen will use the metal oxide force fields to study the structures and reactivities of metal oxide clusters containing 20-30 metal atoms, and to compare to the experimental work of Dellinger. Zhao and Bagayoko (SU) will test the predicted structures and reactivities using DFT-MD.

SD 3: Biomolecular Materials [Ashbaugh (Tulane), Moldovan (LSU)]

Living organisms are composed of the most complex, hierarchically-organized materials known. Proteins, for example, are built from just 20 amino acids and, depending on their sequence, carry out diverse functions including catalysis, signaling, and structural support. The **goal of this SD** is to develop **novel** biomolecular material systems for the encapsulation, delivery, and release of therapeutics to targeted tissues. The **barriers** to achieving these goals are modeling length scales on the order of 10^{-9} to 10^{-7} m and the lack of sufficiently efficient force fields to enable simulations to reach time scales of 10^{-6} to 10^{-3} s required for meaningful predictions. At **present**, all-atom simulations are limited to length scales less than 10^{-8} m and time scales up to 10^{-7} s. Coarse-grained (CG) methods allow simulations that reach 10^{-5} s. A team of 14 faculty members with expertise in multiscale MD, all-atom and CG force fields, and experiment will develop, apply, and validate multiscale methods applicable to biomolecular materials. The **payoff** will be experimentally validated multiscale models that enable the design of novel drug delivery vehicles.

While many drug candidates demonstrate desired therapeutic effects, many also exhibit undesirable solubility, toxicity, or stability *in vivo*. Thus, there is exploding interest in carrier-based delivery methods that combine desired therapeutic effects with specific delivery sites. Two successful approaches include the noncovalent encapsulation of drugs inside self-assembled carriers, such as micelles or liposomes,[90] and the covalent attachment of drugs to polymer scaffolds.[91] Self-assembled carriers offer simple, low cost preparation, but are susceptible to disaggregation *in vivo*. The covalent connectivity of polymer scaffolds affords heartier transport, but requires potentially cost-prohibitive synthesis and drug-attachment/release chemistry. These methodologies are successful, as evidenced by the recent FDA approval of liposomal formulations such as DOXIL for the treatment of Kaposi's sarcoma, and numerous polymer drug candidates in clinical trials, such as OPAXIO for recurring ovarian cancer. Alternately, unimolecular polymeric micelles combine the advantages of single polymer carriers with noncovalent encapsulation, and are expected to expand potential targets. No single delivery strategy will be a panacea for all potential drugs and targets, requiring a multitiered approach to their design.

Molecular and CG simulations will winnow the range of design variables of biodelivery vehicles and circumvent time consuming synthetic and characterization bottlenecks. The Alliance will focus on self-assembled and unimolecular delivery vehicles, covering the range of practical molecular architectures. The modeling of delivery vehicles is inherently multiscale, from molecular-scale bio-specific hydrogen bonding and hydrophobic interactions to nanometer-scale conformational and aggregation state changes. To overcome the **barriers** to these computational objectives, advances in model development must be made. Our coordinated efforts will aim to (1) Develop new inter-atomic interaction potentials using DFT methods developed by Perdew (Tulane) and expand existing force fields (e.g., CHARMM,[92,93] AMBER,[94] GROMOS,[95,96] OPLS,[97] etc.) to systems containing biological and nonbiological molecules; (2) Develop new CG and accelerated simulation strategies linking length and time scales inherent in biological systems. Wick, Chen, and Moldovan (LSU), and Ashbaugh (Tulane) will develop CG models (e.g., expanding the MARTINI[98,99] force field) that preserve structure and thermodynamics between scales. Such techniques have already been developed for modeling homopolymers up to 10^5 g/mol in weight, and will be expanded to heterogeneous biomaterials. In addition, Wick, Chen, Hall, Pratt (Tulane), Rick (UNO), and Ashbaugh will develop advanced hybrid molecular/continuum (HMC) methods to model nonequilibrium transport barriers to delivery. CG models and HMC algorithms will be ported into LAMMPS for broad dissemination; and (3) Develop advanced free energy evaluation strategies across heterogeneous computer networks to calculate differences between macromolecular conformational changes and drug solubilization. Mobley (UNO) will develop these techniques that can be used for both molecular and CG models to reliably translate results across length scales. Specific ***focus*** directions are discussed below. The CTCI visualization group will provide expertise in computing spinors for molecules and other advanced visual analytical techniques. The data management and execution management groups will work closely with SD3 members to reduce the time-to-solution.

SD3, Focus 1: Unimolecular vehicles. Modern polymerization techniques can precisely synthesize nanoscale polymer components. Efficient coupling reactions, such as the Huisgen "click" reaction,[100,101] permit individual polymeric units to be linked to larger, modular assemblies that can be built into supramolecular structures[102-104] for drug and peptide encapsulation[105] that improve their solubility and/or stability *in vivo*. Grayson (Tulane) will synthesize and characterize a modular library of core molecules (Fig. 7) and amphiphilic side chains (including pH sensitive and biodegradable functionalities) to explore encapsulation based on architecture and chemistry.[106] Architectures to be synthesized include linear, star, dendrimer, and macrocycle topologies.[107,108] Encapsulation and hydrophobic dye (pyrene) solubilization in water will be tested using UV-vis. Light scattering will verify the size of the host-guest complexes. Dye-labeled hydrophobic peptide encapsulation will also be investigated. The **goal** of this focus area is to design better unimolecular encapsulation materials.

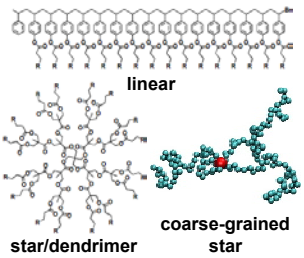


Fig. 5. Linear and star/dendrimer backbones to be synthesized and CG model star snapshot.

Ashbaugh and Bishop (Tulane) will explore the role of architecture and solvent to optimize vehicles for controlled capture and release using hybrid, CG, and acceleration strategies. Molecular simulations will analyze drug solubility in aqueous/nonaqueous solvents and polymer side chain-guest interactions.

Poly(ethylene oxide) oligomers will serve as a prototypical hydrophilic side chain, while poly(caprolactone) and polystyrene oligomers will serve as prototypical hydrophobic side chains. Guests to be studied include pyrene and drug peptides. **Novel** inverse MC simulations will be used to develop CG models (to overcome the time scale **barrier)** whose intra/intermolecular correlations match those of the molecularly detailed simulations described previously.[109] Simulations will allow assessment of the effect of molecular topology (Fig. 5) on encapsulation efficacy. Depending on the topology, different free energies for absorbing/delivering cargo in differing environments will be used to optimize transport efficacy. Computed solubilities will be benchmarked against experiment, and molecular topologies studied by simulation will narrow synthetic targets. A second unimolecular delivery vehicle, halloysite nanotubes, will be studied computationally by Derosa (LATech/Grambling) and experimentally by Lvov (LA Tech, see letter of commitment). Preliminary experimental work has established these nanotubes as effective sustained delivery vehicles.[110,111] The **payoff:** experimentally validated, multiscale models will be developed[112] to predict drug transport from halloysite nanotubes.

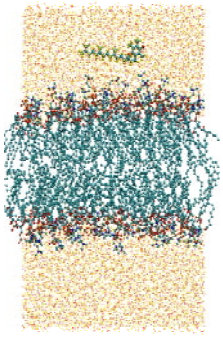


Fig. 6. DMPC bilayer simulation in the presence of α-tocopherol [Moldovan (LSU)].

SD3, Focus 2: Self-assembled delivery vehicles. As a complement to unimolecular carriers, drugs can be entrapped in surfactant assemblies with dimensions less than 100 nm and absorbed via paracellular and transcellular routes in the intestine at rates dependent on the nanoparticle size, surface charge, and hydrophobicity. The **goal** of this focus area is to combine **novel** MD and CG simulation and experimental studies to examine the effects of nanoparticle properties on translocation efficacy through cell membranes. To overcome the time scale **barrier**, both all-atom and CG large-scale MD simulations will be conducted by Moldovan and Nikitopoulos (LSU) and Bishop (Tulane) using GROMACS[113] and LAMMPS[114] to investigate the mechanism(s) of early stage surfactant self-assembly and the release/translocation of drugs through lipid bilayers (Fig. 6). The MD and CG investigations by Moldovan, Nikitopoulos, Bishop, and Ashbaugh are critical for understanding the mechanisms of drug absorption. They can serve to design experiments and to discriminate between mechanisms. The **payoff:** the determination of the optimal conditions (i.e., concentration, pH) under which desired structures are stabilized will be used experimentally to build delivery systems with functionalities targeted to specific applications.

Experimental validation involves the synthesis and characterization of nanoscale delivery systems for improved bioavailability via interfacial phenomena such as the formation of micelles and vesicles,[115] and transport of nanostructures across lipid bilayer membranes, thus emulating cellular uptake. Surfactants and polymers will control nanostructure and functionality. Sabliov (LSU) will use emulsion evaporation to synthesize chitosan/poly(D,L-lactide-co-glycolide) (PLGA) nanoparticles with entrapped α-tocopherol (Chi/PLGA(αT)). The nanoparticles morphology, size distribution, and zeta potentials will be characterized using dynamic light scattering and TEM. The passive transport of Chi/PLGA(αT) nanoparticles through phospholipid bilayers will be investigated using both MD and CG simulations. A biomimetic artificial membrane permeation assay based on dipalmitoyl-phosphatidylcholine liposomes will be used to experimentally assess passive *in vitro* transport of Chi/PLGA(αT). The mechanistic insights revealed by the MD and CG studies will impact directly our fundamental understanding of the role of the Chi/PLGA(αT) nanoparticle characteristics on their transmembrane permeability, ultimately leading to improved delivery protocols.

4.3.4 Research Coordination Plan

The requisite extensive communication among all of the personnel involved in establishing sustainable research collaborations and community building across the State will be a distinctive and transformative feature of this project. These investigators are part of an organizational framework that involves one computational team and the three SD teams, which are tightly integrated with each other. Senior personnel who have significant administrative, oversight, and leadership roles request modest salaries from the proposed budget (see budget justifications). Every project team will involve faculty, students, and postdocs from different campuses. These teams will interact weekly via synchronous HD video. In addition, a **weekly seminar** for all researchers will be scheduled at a rotating site (with speakers from within or outside the project) and broadcast to other sites using synchronous HD video. Following the formal presentation, informal conversations and discussions will take place among the participants across the

State. At the conclusion of these seminars, senior personnel will coordinate projects. The Alliance will produce a monthly electronic newsletter with nuggets describing research progress for internal distribution. These nuggets will help inform and cross-pollinate interactions. **Biannual "all-hands" face-to-face meetings** will be held at rotating sites. After the first year, one of these meetings will feature world-class materials science researchers representing computation, theory, and experiment. Eventually, this will evolve into a sustainable international conference series with participation by the EPSCoR office and participating institutions. A science coordinator will assist the Project Execution Team (PET, see 4.10) to coordinate these activities. The research activities and interactions will develop the collaborative synergy and intellectual capital needed to successfully compete for other funding opportunities. Leveraging of RII funds from other sources and collaborative pursuit of additional funding for the projects will be expected.

An Evaluation & Assessment team (E&A, see 4.10) will conduct regular evaluations of each project's progress towards meeting research milestones as well as the level of participation of project teams in the diversity, workforce, and external engagement aspects of the RII project described in the following sections. These evaluations will be passed to the PET, which will make recommendations to the External Review Board (ERB, see 4.10). These, along with data gathered by an external evaluator (Sec 4.8), will be used by the ERB to make recommendations to the Project Director and the PET for possible adjustments and alterations as needed to achieve the project objectives.

4.3.5 Research Milestones

SD 1: Electronic and Magnetic Materials

Focus 1:

- Develop continuous time QMC solver for 16-way multicore supercomputers (Y 1-2)
- Incorporate Hyper-GGA functionals into common DFT codes including VASP (Y 1-3)
- Develop MSMB solver able to treat multiple correlated orbitals (Y 2-4)
- Port hyperparallel codes to NSF national leadership class machines (Blue Waters) (Y 3-5)

Focus 2:

- Test array of DFT functionals' prediction of metalloporphyrin and ferroelectric properties (Y 1-2)
- Prepare and measure electrical/magnetic properties of metalloporphyrin nanostructures (Y 1-2)
- Develop experimentally validated computational models for porphyrin systems using magnetoresistance and electrical conductance measurements as guides (Y 2-5)
- Develop multiscale models of metalloporphyrin systems using DFT parameters (Y 3-5)
- Predict charge transport in metalloporphyrins and compare with experiments (Y 3-5)
- Prepare organic magnets and ferroelectrics (Y 1-3)
- Predict properties of ferroelectrics using new nonlocal meta-GGA DFT functionals (Y 3-5)
- Develop experimentally validated models of organic magnets and ferroelectrics (Y 3-5)

Focus 3:

- Address the bottlenecks and numerical instabilities in the parquet equations by employing better parallel linear systems solvers and develop multiband parquet codes (Y 1-5)
- Incorporate Ramanujam's advanced tensor rotation and contraction methods (Tensor Contraction Engine) into parquet codes (Y 1-2)
- Use hybrid QMC to address the origin of the QCP and competing order in cuprate models (Y 1-2)
- Study overscreening in pnictide models using new Hyper-GGA functionals (Y 1-3)
- Use methods that combine LDA models obtained from downfolding and DCA/MSMB to study correlation and phonon effects in the pnictides (Y 1-5)

SD 2: Energy Materials

Focus 1:

- Conduct simulation of pore filling in electrochemical capacitors based on nanowire forests (Y 1-2)
- Incorporate chemical processes in electrochemical simulations to study chemical damage at elevated electric potentials (Y 1-3)
- Verify computationally the behavior of quantum capacitance in electrochemical capacitance (Y 2-4)
- Explore additional nanoforest-based capacitor systems (Y 3-5)
- Optimize computational efficiency of *ab initio* MD techniques (Y 1-2)
- Predict catalytic sites in nanotubes (Y 2-5)

- Design, build, and test fuel cells and use results to guide new calculations (Y 3-5)

Focus 2:

- 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 H_2 uptake in bulk alloys (Y 1-2); develop new force fields for new and existing alloys (Y 2-5)
- Develop finite element model to track 3D microstructure evolution and finite difference models for ionic diffusion rates using distances and times provided by experiments (Y 2-4)
- Perform X-ray nanotomography imaging of H_2 uptake in bulk alloys using Argonne's Advanced Photon Source (APS) (Y 1-2), and neutron tomography at NIST (Y 3-5)

Focus 3:

- Develop force fields with environment-dependent charges for one metal oxide system (Y 1)
- Perform computational modeling of water gas shift and Fischer-Tropsch reactions (Y 1-3)
- Perform computational modeling of PCDD/PCDF production on metal oxide clusters (Y 2-3)
- Develop new force fields and study of additional catalytic processes (Y 3-5)
- Validate force field calculations with experimental measurements and DFT calculations (Y 3-5)

SD 3: Biomolecular Materials

Focus 1:

- Synthesize modular library of core molecules and amphiphilic side chains to explore encapsulation based on architecture and chemistry (Y 1-3)
- Develop new inter-atomic interaction potentials and new coarse-grained force fields for systems containing both biological and nonbiological molecules (Y 1-2)
- Develop new hybrid MD/continuum and coarse-grained and accelerated simulation strategies to link length and time scales in biological systems (Y 1-3)
- Use multiscale methods to explore the role of architecture and solvent to optimize supramolecular vehicles for controlled capture and release (Y 3-5)

Focus 2:

- Synthesize, characterize, and assess new transmembrane drug delivery systems (Y 1-3)
- Experimentally utilize, validate, and ultimately improve the newly developed computational models for drug carriers, self-assembling, and translocation through bio-membranes (Y 3-5)
- Use MD and CG methods to study the mechanisms of cellular absorption of drugs (Y 2-5)
- Model new polymer architectures for new carriers, followed by synthesis in the laboratory (Y 4-5)

4.4 Diversity Plan

Women make up 19% of the senior personnel of the Alliance. The racial/ethnic makeup of the Alliance includes 6% African American, 6% Hispanic, and 17% Asian American. Over 21% of the graduate students and 14% of the postdoctoral fellows are women. Underrepresented minorities (URM) of both genders make up 10% of the graduate students and 11% of the postdocs. We propose to dramatically increase the number of URM and women in the Alliance at all levels through the following strategies with the goal of doubling each statistic in five years.

Strategy 1. *Establish a Diversity Advisory Council*. We will create a Diversity Advisory Council (DAC) to advise the Alliance on strategies to achieve gender and racial parity and create an environment in which women and URM thrive and realize their full potential. The council includes national leaders such as UC Berkeley's William Lester (Chair), Betsy Willis of SMU's Gender Parity Initiative,[116] and Sheila Lange, Vice Provost for Diversity at the University of Washington (see letters of commitment). Initially the DAC will have six out-of-state and three in-state members, of which 66% are women, and 55% are African Americans, from some of the best universities in the country. We will also seek the assistance of the DAC members to identify and recruit faculty role models for women and URM at Alliance institutions, and solicit their advice on effective strategies for recruiting URM and women students. There will be some overlap in membership between the DAC and the External Review Board (See Sec. 4.10) to ensure follow-through on their recommendations. ***Milestones:*** DAC established in Y1; annual DAC meetings.

Strategy 2. *Provide financial incentives for pursuing advanced education*. LA-SiGMA will supplement research assistantships at Alliance institutions with $3,750 to entering women and URM students on a

competitive basis, and an additional $3,750 once the students complete their PhD qualifying exams. The recipients will be required to return to their undergraduate institutions to recruit students, thus sustaining the pipeline of students into the graduate programs. These financial incentives will be coupled to aggressive recruiting programs initiated under the guidance of local and national experts (see next item). ***Milestones:*** Reach 30% women and 15% URM graduate students within the Alliance by Y3, and 40% and 20% respectively by Y5.

Strategy 3. *Development of role models*. A great example of what one role model can accomplish is provided by Isiah Warner, Vice-Chancellor of Strategic Initiatives and chemistry professor at LSU, who provided the inspiration and leadership for the Chemistry Department to increase the number of URM chemistry PhD students at LSU from single digits at the time of his arrival in 1992, to an average of 30 by 2000. The American Chemical Society has recognized LSU's Chemistry Department for awarding the highest number of African-American PhDs.[117] We will replicate this success across the State by supplementing departmental start-up packages with LA-SiGMA funds for recruiting new URM and female faculty members with research interests in materials science, and through mentoring current URM and female junior faculty. Professor Jenna Carpenter, Director of the Office of Women in Science and Engineering being established at LA Tech through an NSF ADVANCE grant, will guide the development of support and mentoring networks for women faculty and students. ***Milestones:*** Reach 30% women and 8% URM faculty in LA-SiGMA by the start of Y3; 40% women and 12% URM faculty by Y5.

Strategy 4. *Create/expand pipelines to graduate school*. To encourage URM and women to go beyond undergraduate studies, a 4+1 BS/MS program is being developed between Grambling and LA Tech (Physics/Applied Physics) and a 3+2 dual degree engineering program between Xavier and Tulane has been approved. This project involves three HBCUs—SU, Xavier, and Grambling—with high percentages of URM enrollments and, therefore, a rich talent pool available to us. Xavier ranks first nationally in awarding BS degrees in biology, chemistry, physics, and in the physical sciences to African American students. Jointly funded by NSF EPSCoR and the LA Board of Regents from 1995-2005, a unique Joint Faculty Appointments Program (JFAP) was established whereby faculty members were hired jointly between minority-serving and neighboring majority-white institutions, for example between Tulane/Xavier, LSU/Southern, and LA Tech/Grambling. Four of these JFAP appointees are part of LA SiGMA; they will mentor undergraduate students at the HBCUs and help ease their transition to a graduate program at the partner institution. The Louisiana Community and Technical College System enrolls almost 60,000 students, with African Americans accounting for 36% (Fall 2008 data from BoR). Articulation agreements are being developed to allow two-year college students to transition to four-year institutions and finish their degrees while retaining as many credit hours as possible. ***Milestones:*** At least five students recruited through these pipelines by end of Y2, and 15 by Y5.

4.5 Workforce Development Plan

The Louisiana Workforce Commission reports that in 2007 the State's workforce numbered 1.95 million,[118] with 31% comprised of URMs. This is encouraging in a state in which URMs make up 33% of the population. However STEM disciplines account for less than 4% of the total workforce and, within this group, URMs make up only 16%. LA-SiGMA will address all levels of the educational ladder, including two-year colleges, through a range of training and educational activities, contributing to a well-trained and diverse professional workforce that can support advanced materials research and industries as well as education. Louisiana's two-year college system is relatively young (established in 1999) and has limited relationships with the four-year institutions. The Alliance will make transformative changes to engage this sector in our workforce development plan by leveraging the few existing links and greatly expanding them. Jeff Lynn, the Executive Director of Louisiana FastStart (a workforce solutions provider that works with businesses) will direct efforts to match industry needs with materials science education and training efforts. The LSU LA-SiGMA staff member, requested in the budget, will coordinate these activities, working with staff at each of the institutions (see letters of commitment).

Strategy 1. Middle and high school students will be exposed to computational and experimental materials science projects through campus open house events held once per year at all participating institutions. High school students, nominated by their teachers, will be selected to participate in weeklong summer research workshops to be held in New Orleans (jointly by Tulane, UNO, and Xavier), Baton Rouge (jointly by LSU and SU), and Ruston (jointly by LA Tech and Grambling). These workshops will be

held in parallel with the research experiences for teachers (RET) discussed in Strategy 2. ***Milestones:*** 100 open house attendees in Y1, increasing in Y2 and beyond; 40 students in summer workshops in Y1, increasing in Y2 and beyond.

Strategy 2. Grades 6-12 and two-year college teachers will be offered summer RET programs held annually in New Orleans, Baton Rouge, and Ruston, as in Strategy 1. The RET program will focus on discovery-based modules designed for classroom use. Additional workshops will address specific techniques for including content in discovery-based courses. In the first year, a pilot program at Baton Rouge Community College (BRCC) will develop computational materials science modules for use in BRCC's developing engineering program (see letter of commitment). In subsequent years, this program will be expanded to other disciplines and two-year colleges. ***Milestones:*** 20 RET participants (as budgeted) each year; use of modules in classroom (tracked through follow-up visits to classrooms); expansion of pilot program in Y2 and beyond.

Strategy 3. Multiple programs will serve **two-year college students**. Modeling the collaboration between Chemical and Biomolecular Engineering at Tulane and the Process Technology program at Nunez Community College, we will develop short courses to train two-year and technical college students to use sophisticated materials research instrumentation, such as NMR, XRD, SEM, and AFM. In the first year of the grant, LA Tech will offer a pilot course in materials characterization using X-ray diffraction to regional community college students. In the following years, course offerings will be expanded to other instrumental techniques. The Beowulf Boot Camp for high school students and teachers, conducted annually by Thomas Sterling (the father of the beowulf supercomputer architecture) at LSU,[119] will be expanded to include the application of HPC methods to materials science and taught to BRCC students in a pilot program during the first year. In subsequent years, the two pilot programs will be expanded to the other participating institutions. Students who become interested in furthering their education as a result of these initiatives will be recruited into undergraduate programs in four-year institutions. ***Milestones:*** Initiation of short-course pilot programs in Y1 and expansion in Y2 and beyond; five two-year college participants each year in Beowulf Boot Camp; expansion of 2+2 programs to other LA-SiGMA institutions by Y3.

Strategy 4. Undergraduates at **four-** and **two-year** institutions will participate in summer research experiences for undergraduates (**REU**) programs focused on computational and experimental materials science at all LA-SiGMA institutions. Students will be supervised by a computational researcher and co-advised by an experimentalist and attend weekly lectures with topics such as project planning, literature review, scientific writing, research presentation, and ethical conduct. Also, training in HPC and CyberTools will be scheduled regularly. Studies show that early involvement of undergraduate students in research increases their retention rates.[120] ***Milestones:*** 30 REU participants (as budgeted) each year; 50% of participants will pursue higher education.

Strategy 5. Graduate students will join a transformative educational experience in materials science. A core set of graduate level courses (three in the first year, six more in subsequent years) in computational science, multiscale modeling methods, advanced experimental techniques, and other topics will be developed and broadcast throughout the State using synchronous HD video. The letters of commitment demonstrate the dedication of each participating institution to this educational effort. These courses will be integrated into existing and new graduate curricula on each campus. LA-SiGMA will also cover the costs for graduate students to attend the "Supercomputing Education Program,"[121] which is part of Oklahoma's EPSCoR RII program. ***Milestones:*** Enrollments in new courses (at least 40 statewide); incorporation into graduate curricula on two campuses by Y2, others by Y3.

Strategy 6. Postdocs[1] and **graduate students** will also participate in a unique program that trains postdocs in the use of best practice teaching methods based on Michigan State's Faculty Institutes for Reforming Science Teaching (FIRST) project.[122] Undergraduates, graduate students, and postdocs will take part in national labs and industrial internships (see letters of commitment) at Los Alamos, Sandia, and Pacific Northwest National Labs, and at Renewable Fuels, Carbon Capture Energy Technologies, and Radiance Technologies. ***Milestones:*** Participation in effective teaching workshops; five internships and extended visits each year.

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1 A comprehensive postdoctoral mentoring program is provided in Supplementary Documents, as required.

4.6. Cyberinfrastructure Plan

Strategy 1. *Leverage LONI facilities*. LONI, envisioned by Ed Seidel (the first chief scientist of LONI, now Director of NSF's Office of Cyberinfrastructure), provides a world-class CI to Louisiana. The LONI Management Council (MC) reports to the BoR and consists of 15 representatives of public and private universities, two-year and technical colleges, Division of Administration (State CIO), and Louisiana Dept. of Economic Development. The MC and the Louisiana EPSCoR Committee work to ensure their activities are coordinated and integrated to advance the State's CI. The MC, which played a key role in securing ongoing funding from the State for CI improvements, supports major CI funding initiatives pursued by LONI member institutions. The MC allocates some of LONI's HPC resources to specific research projects. As noted in the attached letter, the MC commitment of at least 10% of LONI's resources, which is equivalent to 4.5M service units, is evidence of their strong support for the proposed project.

LONI's 40-Gbps network connects the IT and materials science centers of excellence at Louisiana's research universities, providing the linkages that are essential for effective collaborative research in computational materials. LONI's 85 TFLOPS of HPC are distributed across the State to support broader ownership and utilization of these resources. The synchronous HD video facilities in most of Louisiana's major research centers will foster regular and seamless communications between the research teams. LONI's Phase 2 network deployment extended connectivity to almost all four-year institutions, as well as two-year and technical colleges, to enable broad outreach to and engagement of all of Louisiana's higher education community. Louisiana's CI plans also include targeted investments across the State in the hiring and training of researchers in computational sciences—researchers who understand the evolution of advanced computing tools and the science challenges that stretch the limits of existing analytical and experimental resources. These computational scientists have significantly improved LONI's hardware and software tools; these tools will be important in advancing the materials science challenges of this project. **Milestones**: At least 60% of the 4.5M SU's assigned to SD teams by 2nd quarter, 100% assigned by end of Y1.

Strategy 2. *Build upon the CCT and Cybertools RII*. Another significant resource available to the Alliance is the CCT, LSU's Center for Computation and Technology, which played an integral role in the development of LONI's CI and is a major resource for the proposed project. CCT scientists will adapt many of the "CyberTools" developed through the current RII project to the needs of the Alliance. For example, Petashare, a statewide mountable rapid access file system with archival capabilities, will be used to share and archive scientific data using common data formats for Monte Carlo (Towhee), MD (LAMMPS, CHARMM, AMBER, GROMACS, NAMD, which have compatible file formats or converters), and for the archival of DFT output (VASP, Guassian03, NWChem, GAMES). Petashare allows researchers to produce data at one site and analyze it at another. CyberTools also provides a common visualization environment utilizing a common data format via the Petashare system.

The CTCI group will work with the CI Development (CyD) group at CCT, participating campus HPC divisions, and the LONI Management Council to meet the research requirements of the project. LA-SiGMA will play a major role in guiding the utilization and future evolution of the computational environment provided by LONI, and will also work with LONI and CyD to ensure that each site has compatible synchronous HD video access. High definition communication and collaboration equipment are essential for teaching; i.e., so students can clearly see the white board and interact effectively with participants at the remote site. **Milestones**: All LA-SiGMA sites with HD video access by Y2. Twenty-five percent of SD researchers using Cybertools by Y5.

Strategy 3. *Migrate to National Leadership Class Computing*. The CTCI team is also positioning Louisiana to leverage future CI development. The advent of hyperparallel, multicore, heterogeneous, and low power architectures presents both a tremendous opportunity for new scientific discovery and the challenge of training Louisiana researchers to effectively use these machines. To advance training in these areas, members of different scientific focus areas will share students with computer scientists specializing in HPC, including Ramanujam, Leangsuksun, and Sterling. To help train these students, we will purchase nodes of multicore, low power, and heterogeneous systems so the students can learn to program before such machines become available on the TeraGrid. These machines will also be used to teach courses offered statewide via synchronous HD video. The CTCI team will work with the computational teams to help more experienced researchers expand their programs beyond LONI to national-leadership class re-

sources such as TeraGrid Kraken, and to utilize the next generation of computer architectures (BlueWaters). **Milestones**: More than three codes ported to national leadership class machines by Y3.

Strategy 4. *Expand impact of LA-SiGMA*. To increase the impact of the computational formalisms, algorithms, and codes we develop, we will publish their details in journals such as *Computer Physics Communications*. We will release the associated software under a modified open source license* in which each user is required to cite these publications. A modular software engineering approach will be used in development of the project software. Use of a component standard such as the Common Component Architecture (CCA)[123] will be evaluated for appropriateness for the code developed in this project. The web interface will leverage existing grid-portal development frameworks and standards to ensure interoperability with other web services.[124] All software will be managed and maintained using a version control system. Components will undergo unit testing for both correctness and performance, and a defect and feature tracking system will be used for managing error reporting and maintenance of all released software. **Milestones**: Four codes, with full documentation, publicly available by Y3.

4.7 External Engagement Plan

We have designed a multi-institutional external engagement program that will provide a well-prepared and competent workforce and educate and engage the public. Through the use of face-to-face meetings and CI tools such as synchronous HD video, our program will provide for efficient collection and dissemination of information between participants, the K-12 community, two-year colleges, and the general public.

Strategy 1. *Leverage multiple avenues to engage the general public*. The Alliance will communicate scientific advances and discoveries to the general public by (1) providing guests to Louisiana Public Broadcasting (LPB) and other television programs; (2) public lectures delivered by Alliance members in computational thinking, parallel computing, and computational materials science; (3) leveraging NSF's other investments, such as education kiosks at the Exploratorium of the Laser Interferometer Gravitational Observatory (LIGO) located in Livingston Parish; and (4) lectures on the promises and challenges of multiscale materials modeling offered to local and regional industry, facilitated by an Industrial Liaison Team (ILT). ***Success criteria:*** At least one LPB appearance per year by a LA-SiGMA member; at least one public lecture delivered each quarter; at least one lecture delivered to industrial audiences each quarter.

Strategy 2. *Create a web portal for distribution of project deliverables*. The Alliance will create a web portal to provide (1) archived videos of public lectures, (2) seminars delivered by invited seminar speakers, (3) course material developed by Alliance members, and (4) classroom lectures for the new courses developed for statewide delivery. ***Success criteria:*** Web portal created in Y1; traffic increases 20% annually.

Strategy 3. *Create a repository and version control system for code development and distribution*. The computational tools created by the Alliance will be archived using an integrated SVN, wiki, and Bugzilla (or other bug tracking software) system in addition to annual code releases with accompanying documentation. The Common Component Architecture (CCA) mentioned in Sec. 4.6 will also be used to ensure interoperability of code modules. ***Success criteria:*** SVN created in Y1; maintained and upgraded in Y2-5; 100 code downloads per year starting Y3.

Strategy 4. *Leverage cyberinfrastructure to facilitate communication*. The jurisdiction has invested in IOCOM distributed collaboration systems at all participating campuses, consisting of integrated video conferencing systems that are compatible with the existing Access Grid network. The proposed budget includes funds for HD Polycom stations to supplement existing infrastructure to facilitate extensive communication both within the Alliance as well as international partners. ***Success criteria:*** Polycom HD stations purchased and installed at participating institutions in Y1.

Strategy 5. *Use Newsletter/Brochures/Highlights to publicize Alliance activities*. The LA EPSCoR monthly newsletter highlights the role played by LA EPSCoR in promoting the development of the State's science and technology resources through partnerships involving its universities, industry, and government. The

* Our license will allow full and open use, modification, and extension of our software products, such as described at: http://opensource.org/licenses/ with the minimal restrictions to protect the jurisdiction's ownership rights,

newsletter is distributed by mail to 400 individuals, including State legislators, and electronically to more than 720 email addresses, which includes federal funding agencies. ***Success criteria:*** At least two LA-SiGMA highlights featured in EPSCoR newsletter each year; at least one story picked up by regional/national press.

Strategy 6. *Create formal mechanisms for engagement with NSF*. An annual meeting with representative program officers from NSF and other federal funding agencies will provide a forum for faculty from all participating institutions to learn about institution-appropriate funding opportunities. Michael Khonsari, the State EPSCoR Project Director, will coordinate communication with the NSF EPSCoR office. Synchronous HD video conferencing is available at the EPSCoR office to interact with NSF. ***Success criteria:*** Regular interactions with NSF; at least three research highlights reported to NSF annually.

Strategy 7. *Establish new national and international collaborations*. The Alliance will leverage partnerships with national labs (see Sec. 4.5) to promote national collaborations to benefit students and faculty. We will also leverage our extensive collaborations with international partners (Moreno's PIRE program between LSU and seven partners throughout Germany and Switzerland, the collaboration between the Italian National Nanotechnology Labs and LA Tech "Progetto Bilaterale Italia-USA," etc.) to provide educational experiences for our students and faculty. The code distribution (Strategy 3) will also help develop new partnerships across the world. ***Milestones:*** 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.

Strategy 8. *Create mechanisms for internal communications*. The Alliance will host biannual all-hands "face-to-face" meetings to share information and data. These meetings will provide a mechanism for interaction with the Diversity Advisory Committee (DAC), Industrial Liaison Team (ILT), and External Review Board (ERB) as well. ***Milestones:*** Full participation in biannual meetings.

To support these activities, a full-time external engagement and workforce development coordinator and a support-staff member will be hired at LSU. A staff person who will support external engagement activities as well as evaluation and assessment (see Sec. 4.8) will also be hired at LA Tech.

An additional external engagement avenue that will be utilized by the Alliance is the "Speaking of Science Speakers Bureau" (SoS) administered by the State EPSCoR Office. The LA EPSCoR SoS program for K-16 provides students in public and private schools exposure to the best researchers in the State. Its purpose is to increase public awareness of exciting R&D in Louisiana, spark the interest of students in S&E professions, and showcase the excellence of Louisiana's leading S&E faculty and professionals. Speakers are available free of charge to students, educators, and general audiences throughout Louisiana on a wide variety of topics. The Alliance will regularly provide speakers to participate in this program and thus inform the K-16 community of the research and education activities being conducted by Alliance members. ***Success criteria:*** At least two LA-SiGMA speakers per year.

4.8 Evaluation and Assessment Plan

A comprehensive Evaluation and Assessment (E&A) plan will be created based on (1) the research milestones provided in Sec. 4.3.5; (2) the milestones and success criteria for each strategy discussed in Secs. 4.4, 4.5, 4.7, and 4.9.2; and (3) global metrics designed to measure the impact of the project on the jurisdiction's S&T enterprise. The Evaluation & Assessment Team (see 4.10) 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 data to make course corrections and improvements.

1. Data collection: A web-based data collection system will be implemented to simplify the frequent data collection required for effective assessment of project activities. The PIs of each Science Driver (SD) team 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 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.

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

3. 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 project. 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.

A staff member will coordinate the internal data collection and analysis so that the E&A committee (see 4.10) can provide timely feedback to project teams and recommend course correction if necessary. An external evaluator who has many years of experience with E&A of complex projects will be hired by the Alliance. The evaluator will help develop instruments for formative assessment, and will be involved in all aspects of assessment for the duration of the project. The ERB (see Sec. 4.10) will use all assessment data and conduct a thorough annual review of the entire project. The conclusions drawn will be used by the ERB to make recommendations to the Project Director and the PET for possible adjustments and alterations as needed to achieve the project objectives. Some of the global metrics used to assess the impact of the project on the jurisdiction's S&T enterprise are tabulated below.

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 two-year colleges entering degree programs at four-year institutions 3. Percentage of two-year college teachers in RET programs.	1. 100% 2. 25% 3. 15%

4.9 Sustainability Plan

The proposal creates a set of "pillars of sustainability" that will allow the combined efforts of this proposal to continue beyond the life of the grant. These pillars include seed funding, human resource development, and post-RII extramural funding, a description of which follows.

4.9.1 Seed Funding and Emerging Areas. Seed funding is essential to sustain the next generation of Louisiana faculty and promote research innovation. The LA EPSCoR office will administer several seed funding programs promoting all areas of inquiry, thus greatly enhancing the impact of this project. These grants will be competitively awarded through a peer-review process utilizing experts external to Louisiana, using the pledged cost-commitment.

Pilot Funding for New Initiatives (Pfund) program: provides seed-grant research funding for the State's tenure-track science and engineering junior faculty members seeking to demonstrate innovative or novel concepts that could result in attracting federal funds. The review criteria are: (1) Does the proposed research project appear to be technically and scientifically sound? (2) Do the proposed research and supporting materials provide convincing evidence of the potential to attract federal funding, i.e., through future proposal submissions to federal agencies? (3) What is the likelihood that the proposed research will be fundable by NSF?

Planning Grants for Major Initiatives program: provides assistance to teams preparing multidisciplinary research and/or education proposals to large scale (at least $1M) federal initiatives in emerging areas. Review criteria for this program include (1) a viable, multidisciplinary team of investigators; (2) a clearly defined scientific and technical focus; (3) a core theme with strong federal funding potential; (4) a well conceived plan for developing a major initiative proposal; and (5) adequate institutional resources and support.

Links with Industry and National Labs (LINK) program: this initiative helps develop a diverse, internationally competitive and engaged workforce of scientists and engineers by providing opportunities for Louisiana faculty, postdoctoral researchers, and graduate and undergraduate students to visit and conduct research at national laboratories, research centers, or industrial facilities (see letters of commitment). These interactions are often a precursor to obtaining follow-up project funding. Review criteria are: (1) soundness of the proposed research; (2) potential benefit to the applicant's research and education program; (3) potential for increased research productivity, e.g., attracting federal funds, production of publications, etc.; and (4) appropriateness of linkage between applicant and partnering facility and institutional or other support.

SBIR/STTR Phase Zero Grants: this successful program supports the development of projects with economic potential by offering "Phase Zero" awards that assist small businesses in preparing for and successfully competing for SBIR/STTR Phase I proposals. Encouraging high-tech small business development is particularly important considering the post-Katrina environment in New Orleans and the region.

Industrial Partnerships for Emerging Opportunities: a new program that will allow university researchers and industry partners to pursue R&D endeavors that have potential for further long-term investigation and funding from other sources. These partnerships could involve projects to solve problems of immediate interest to industry, or projects that could lead to new inventions, intellectual property, and spin-off companies.

Travel Grants for Emerging Faculty (TGEF): this program aims to assist emerging faculty (tenure-track but untenured) in the S&T disciplines by providing travel funds needed to further their research and build strong collaborations. TGEF provides funds to untenured faculty to visit a federal funding agency program officer and discuss their research proposals, and to present invited talks at national or international meetings.

Louisiana Faculty Expertise Database and Funding Opportunities Search/Alert System (FED): is a tool faculty can use to identify sources of extramural funding. FED utilizes InfoEd's SPINPlus funding opportunities database to advertise the expertise of State researchers and facilitates collaborations with universities and industry. It also matches faculty profiles against the latest funding opportunities and alerts faculty by email with detailed descriptions of programs. Over 3,200 Louisiana faculty have subscribed to this service.

4.9.2 Education and Human Resources Development. Human infrastructure is the central component of LA-SiGMA. The educational programs and research collaborations described in Secs. 4.4, 4.5, and 4.7 are *by design* intended to create a sustainable human infrastructure. The rationale for the education and HRD activities listed below is the recognition that building and sustaining intellectual infrastructure is the most effective way for the State to progress economically and to raise the standard of living of its citizens.

Faculty recruitment. Additional faculty will be recruited to expand and buttress the efforts of LA-SiGMA. Tulane is recruiting an endowed chair in materials science for its newly created Division of Physical and Materials Science. The College of Basic Sciences at LSU will hire an expert in molecular dynamics (MD) (see attached letter of commitment) who will drive the development of the next generation of MD algorithms. LA Tech's College of Engineering & Science will give highest priority to faculty candidates who will strengthen LA-SiGMA in its future hiring plans. These hires will be coordinated so that the diversity milestones described in Sec. 4.4, Strategy 3 are met. **Milestones:** Reach 30% women and 8% URM faculty in LA-SiGMA by the start of Y3; 40% women and 12% URM faculty by Y5.

Distributed Research Experiences for Students. Modeled on a similar initiative sponsored by the Computer Research Association's Committee on the Status of Women in Computing Research, the LA EPSCoR office will establish a statewide network to match promising undergraduates (with a priority on women and underrepresented groups) with faculty mentors for summer research experiences at the faculty member's home institution. Student/faculty pairs selected by a review panel will receive funding to facilitate the undergraduate research experience. **Milestones:** Provide 50 student research experiences per year.

Workforce Training. The training activities outlined in Sec. 4.5 and external engagement of the general public (Sec. 4.7) will be sustained by incorporating the successful elements into future grant proposals prepared by Alliance members. In addition, LA-SiGMA will compete for various federal training grants such as IGERT, VIGRE and GK-12 as well as the graduate fellowships funded by the BoR to sustain these activities. Involvement in K-12 education/training activities is a requirement for BoR graduate fellows. **Milestones:** LA-SiGMA IGERT in Y2 and other training grants pursued in Y3-5.

Statewide EPSCoR Workshops and Conferences. LA EPSCoR will sponsor statewide and regional conferences, including grant-writing workshops featuring nationally recognized experts who can assist faculty in identifying grant opportunities and planning and writing proposals. LA EPSCoR will also sponsor meritorious conferences with research themes that complement our core research initiatives. The State EPSCoR Committee is fully engaged in the planning of major state/regional conferences. During the project period, one of the biannual "all-hands" meetings of LA-SiGMA will evolve into an annual conference with national and international participation and sustained by the participating institutions. **Milestones:** One statewide conference annually; up to four grant-writing workshops annually; and up to three theme-specific (such as entrepreneurship and innovation, diversity, and emerging science topics) workshops/conferences per year.

4.9.3 Post RII Extramural Funding. The proposal creates a set of "pillars of sustainability" that will allow the combined efforts of this proposal to continue beyond the life of the grant.

Centers. A short-term goal of this proposal is building groups with expertise in a number of thematic research areas that can serve as the basis for continued collaborative group proposals ultimately resulting in a research center. Initial efforts will focus on joint proposals and smaller group proposals like the IGERT program. Success here will build towards larger centers (MRSEC, ERC, NSEC, STC, etc.) by the end of the EPSCoR-RII grant period.

Collaborations. Emphasis of research projects funded by the EPSCoR-RII will be towards building new interdisciplinary and interinstitutional collaborations. The goal is to build a successful network of collaborations that can pursue larger group and center proposals to sustain funding. The renewal application for the NSF-funded PIRE program at LSU (PI: Moreno) will propose to expand the program to other LA-SiGMA institutions. In addition, LA-SiGMA researchers will sustain international collaborations through the "Materials World Networks" program of NSF and other opportunities.

4.10 Management Plan

Since its establishment in 1987, LA EPSCoR has existed as a fully integrated entity within the LA Board of Regents (BoR), the coordinating authority for higher education in Louisiana. Michael Khonsari, EPS-

CoR Project Director (PD) and BoR Associate Commissioner for Sponsored Programs Research and Development, is responsible for the overall management of this RII project. He implements and executes the directives of the 21-member statewide EPSCoR Committee and serves as liaison between NSF, the EPSCoR Executive Committee, and the Project Execution Team. The EPSCoR Committee meets formally a minimum of twice yearly, while its elected Executive Committee meets much more frequently. A full-time, highly experienced professional staff assists the PD and the EPSCoR Committee with fiscal and contract management, database administration, external engagement, statewide outreach coordination, and reporting and communications activities. This organization has successfully managed all past EPSCoR awards including the current RII cooperative agreement.

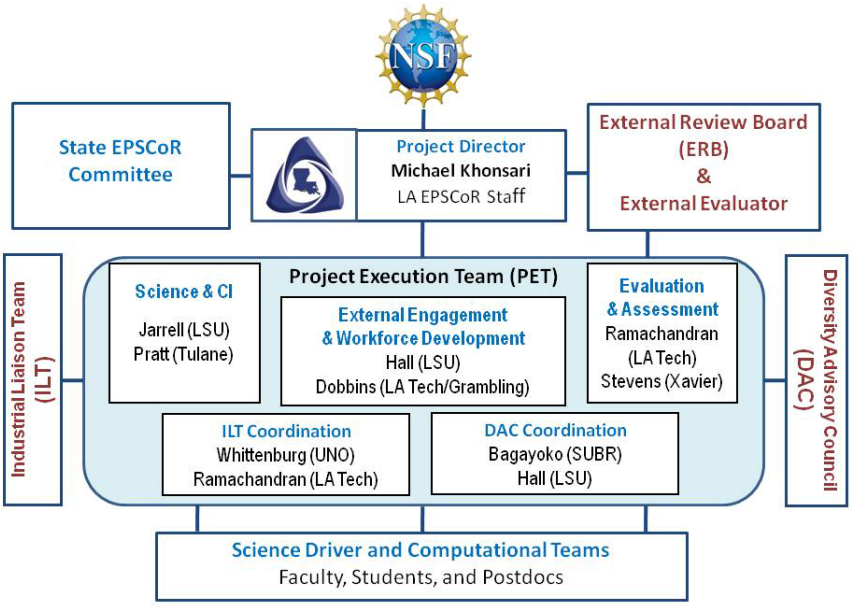

Fig. 7. LA-SiGMA Management Structure

The management structure (Figure 7), which features several interconnected teams described below, is designed to effectively implement and assess the project goals, promote project-wide participation in leadership, and ensure effective communications among universities.

The **Project Execution Team (PET)** will oversee the day-to-day activities of the project and provide direction and guidance to project participants in each of the science driver and computational teams. The eight-member PET, which is comprised of the science leads from each participating institution, includes two females and two African Americans. The PET members are all experienced scientists with the requisite management skills to lead large multidisciplinary projects. They will play vital roles in ensuring effective communications between and within institutions. The co-leads will assume leadership responsibilities to ensure a smooth succession of leadership, should it become necessary. The PD will meet with the PET every other month, at a minimum. Each member will be responsible for defined tasks as follows:

- **Science & Cyberinfrastructure** (lead: Mark Jarrell, LSU; co-lead: Lawrence Pratt, Tulane) will focus on evaluating and monitoring multi-institutional collaborative research projects such as those described in Sec. 4.3 and the statewide cyberinfrastructure plan described in Sec. 4.6. The science coordinator will assist this committee to coordinate statewide activities.
- **External Engagement & Workforce Development** (lead: Randall Hall, LSU; co-lead: Tabbetha Dobbins, LA Tech/Grambling), will oversee the proposed external engagement, diversity, and workforce development activities as outlined in Secs. 4.4, 4.5, and 4.7.
- **Evaluation & Assessment** (lead: Bala Ramachandran, LA Tech; co-lead: Cheryl Stevens, Xavier) supported by one full-time staff and an internal evaluator, will assess all activities of the other two committees, as described in Sec. 4.8, and will also be responsible for providing assessment data to the External Review Board.
- The **Diversity Advisory Council (DAC)** (see Sec. 4.4) will be coordinated by Diola Bagayoko, SU and Randall Hall, LSU. Council members include nationally known experts in materials science as well as individuals with national reputations for promoting ethnic and gender diversity in STEM disciplines. The DAC will interact regularly with the PET by video conference and other means to assess progress towards achieving project diversity goals and to provide guidance and feedback on mechan-

isms to improve success. DAC members will also attend at least one of the biannual meetings to interact with the External Review Board as well as faculty, postdocs, and students in the Alliance.

- An **Industrial Liaison Team (ILT)** will be coordinated by Scott Whittenburg, UNO and Bala Ramachandran, LA Tech. The ILT will be composed of the intellectual property/industrial liaison officers from LSU, LA Tech, and Tulane. Jeff Lynn of the Louisiana Economic Development agency's FastStart™ program and Roy Keller of the LA Business and Technology Center will assist the PET in maximizing the economic impact from the project (see letters of commitment for ILT member participation). The ILT will identify industry and government partners who can participate in the research projects and capitalize upon the tools and other research outcomes. The ILT will meet regularly and organize at least one workshop annually that brings together the research teams and industry partners to explore collaborative projects.

An **External Review Board** (ERB) composed of nationally known experts in the research topics, diversity, workforce development, external engagement, and assessment, as well as an external evaluator, will conduct comprehensive reviews of program activities, including annual site visits. The ERB will review evaluation and assessment data provided by the E&A leads (see 4.8), and provide objective guidance, feedback, and recommendations to the PD and PET to ensure that program goals and objectives are being met. The LA EPSCoR Executive Committee will also meet with the ERB to ensure that broader goals of the jurisdiction are being achieved, recommend avenues to improve and further advance the project, and to resolve any obstacles or conflicts that may occur.

Biannual "all-hands" face-to-face meetings will be used for coordination and identification of new collaborations. The DAC and ILT will participate in the biannual all-hands meetings. The ERB will attend at least one of these biannual meetings to evaluate all aspects of the project. The PET leads will be responsible for communicating with project teams in accordance with Sec. 4.3.4.

In summary, by leveraging current facilities, we will build statewide interdisciplinary research collaborations involving computational and computer scientists, applied mathematicians, theorists, and experimentalists. We will build a sustainable interinstitutional computational materials science graduate program. Thus, LA-SiGMA addresses the dominant barrier to success in Louisiana, the lack of critical intellectual mass at any one campus, to bring about a transformative and sustainable impact in computational materials research, and education, and position the State to compete for and secure the first federally funded center of excellence for simulation-guided materials applications in Louisiana.

Table A. Research Support Levels Requested from NSF

Awardee	Year 1	Year 2	Year 3	Year 4	Year 5	Total	%
LSU - Lead Institution[(a)]	$ 950,647	$ 989362	$ 993,136	$ 887,201	$ 869,524	$ 4,689,930	23.4%
Tulane	$ 553,174	$ 536,475	$ 549,687	$ 557,004	$ 556,575	$ 2,752,915	13.8%
LA Tech/ Grambling[(b)]	$ 613,606	$ 598,768	$ 612,490	$ 621,775	$ 621,251	$ 3,067,890	15.4%
UNO	$ 401,834	$ 382,684	$ 391,506	$ 396,459	$ 396,023	$ 1,968,506	9.8%
SU	$ 386,205	$ 366,980	$ 375,262	$ 379,997	$ 379,725	$ 1,888,169	9.4%
Xavier	$ 234,034	$ 236,666	$ 241,242	$ 243,409	$ 243,222	$ 1,198,573	6.0%
BoR[(c)]	$ 860,500	$ 889,065	$ 836,617	$ 914,155	$ 933,680	$ 4,434,017	22.2%
TOTAL	**$ 4,000,000**	**$ 4,000,000**	**$ 4,000,000**	**$ 4,000,000**	**$ 4,000,000**	**$20,000,000**	**100%**

(a) Includes equipment to be purchased by LSU and installed for use by all institutions.
(b) Includes salaries for the two Grambling participants who hold joint appointments between the two institutions (See Sec. 4.4; Strategy 4) and undergraduate research support at Grambling.
(c) BOR total includes support for LA EPSCoR office, LINK, Planning Grants, workshops and conferences, evaluation and assessment.

References

(1) http://www.er.doe.gov/bes/reports/files/CTF_rpt.pdf, last access date: June 23, 2009

(2) http://www.er.doe.gov/bes/reports/files/CG_rpt.pdf, last access date: June 23, 2009

(3) Glatzmaier, G. A.; Roberts, P. H. Rotation and Magnetism of Earth's Inner Core. Science, 274, 1887-1891, 1996.

(4) Rempel, M.; Schussler, M.; Cameron, R. H. Penumbral Structure and Outflows in Simulated Sunspots. Science, 325, 171, 2009.

(5) http://www.nsf.gov/pubs/2007/nsf0728/nsf0728.pdf, last access date: June 9, 2009

(6) http://www.ncsa.illiniois.edu/News/Stories/BWscience/, last access date: July 21, 2009

(7) Cai, W.; Kalos, M. H.; de Koning, M.; Bulatov, V. V. Importance Sampling of Rare Transition Events in Markov Processes. Physical Review E, 66, 046703, 2002.

(8) de Koning, M.; Cai, W.; Sadigh, B.; Oppelstrup, T.; Kalos, M. H.; Bulatov, V. V. Adaptive Importance Sampling Monte Carlo Simulation of Rare Transition Events. The Journal of chemical physics, 122, 074103, 2005.

(9) Perdew, J.; Burke, K.; Ernzerhof, M. Generalized Gradient Approximation Made Simple. Physical Review Letters, 77, 3865-3868, 1996.

(10) Tao, J. M.; Perdew, J. P.; Staroverov, V. N.; Scuseria, G. E. Climbing the Density Functional Ladder: Nonempirical Meta-Generalized Gradient Approximation Designed for Molecules and Solids. Physical Review Letters, 91, 146401, 2003.

(11) Perdew, J. P.; Ruzsinszky, V. N.; Csonka, G. I.; Constantin, L. A.; Sun, J. Workhorse Semilocal Density Functional for Condensed Matter Physics and Quantum Chemistry. Physical Review Letters, 103 026403, 2009.

(12) Zhao, Y.; Truhlar, D. The M06 Suite of Density Functionals for Main Group Thermochemistry, Thermochemical Kinetics, Noncovalent Interactions, Excited States, and Transition Elements: Two New Functionals and Systematic Testing of Four M06-Class Functionals and 12 Other Functionals. Theoretica Chemica Acta, 120, 215-241, 2008.

(13) van Duin, A. C. T.; Dasgupta, S.; Lorant, F.; Goddard, W. A. Reaxff: A Reactive Force Field for Hydrocarbons. Journal of Physical Chemistry A, 105, 9396-9409, 2001.

(14) Metzner, W.; Vollhardt, D. Correlated Lattice Fermions in D=Infinity Dimensions. Physical Review Letters, 62, 324-327, 1989.

(15) Mueller-Hartmann, E. Correlated Fermions on a Lattice in High Dimensions. Zeitschrift fur Physik B, 74, 507-512, 1989.

(16) http://www.itrs.net/Links/2007ITRS/Home2007.htm, last access date: June 12, 2009

(17) Isaacman, S.; Kumar, R.; Barco, E.; Kent, A.; Canary, J.; Jerschow, A. Critical Examination of Fe8 as a Contrast Agent for Magnetic Resonance Imaging. Polyhedron, 24, 2691-2694, 2005.

(18) Rodriguez, E.; Roig, A.; Molins, E.; Arus, C.; Quintero, M. R.; Cabanas, M. E.; Cerdan, S.; Lopez-Larrubia, P.; Sanfeliu, C. In Vitro Characterization of an Fe-8 Cluster as Potential MRI Contrast Agent. Nmr in Biomedicine, 18, 300-307, 2005.

(19) Pope, M.; Swenberg, C. Electronic Processes in Organic Crystals and Polymers, Oxford University Press, New York, NY1999.

(20) Malliaras, G.; Friend, R. An Organic Electronics Primer. Physics Today, 58, 53-58, 2005.

(21) Dagotto, E. Complexity in Strongly Correlated Electronic Systems. Science, 309, 257-262, 2005.

(22) Andersen, O.; Saha-Dasgupta, T. Muffin-Tin Orbitals of Arbitrary Order. Physical Review B, 62, 16219-16222, 2000.

(23) Kotliar, G.; Savrasov, S.; Haule, K.; Oudovenko, V.; Parcollet, O.; Marianetti, C. Electronic Structure Calculations with Dynamical Mean-Field Theory. Reviews of Modern Physics, 78, 865-951, 2006.

(24) Hettler, M. H.; Tahvildar-Zadeh, A. N.; Jarrell, M.; Pruschke, T.; Krishnamurthy, H. R. Nonlocal Dynamical Correlations of Strongly Interacting Electron Systems. Physical Review B, 58, R7475-R7479, 1998.

(25) Hettler, M. H.; Mukherjee, M.; Jarrell, M.; Krishnamurthy, H. R. Dynamical Cluster Approximation: Nonlocal Dynamics of Correlated Electron Systems. Physical Review B, 61, 12739-12756, 2000.

(26) Jarrell, M.; Krishnamurthy, H. R. Systematic and Causal Corrections to the Coherent Potential Approximation. Physical Review B, 63, 125102, 2001.

(27) Maier, T.; Jarrell, M.; Pruschke, T.; Hettler, M. H. Quantum Cluster Theories. Reviews of Modern Physics, 77, 1027-1080, 2005.

(28) Hirsch, J. E.; Fye, R. M. Monte-Carlo Method for Magnetic-Impurities in Metals. Physical Review Letters, 56, 2521-2524, 1986.

(29) Jarrell, M.; Maier, T.; Huscroft, C.; Moukouri, S. Quantum Monte Carlo Algorithm for Nonlocal Corrections to the Dynamical Mean-Field Approximation. Physical Review B, 64, 195130, 2001.

(30) Rubtsov, A.; Savkin, V.; Lichtenstein, A. Continuous-Time Quantum Monte Carlo Method for Fermions. Physical Review B, 72, 035122, 2005.

(31) Troyer, M.; Wiese, U. Computational Complexity and Fundamental Limitations to Fermionic Quantum Monte Carlo Simulations. Physical Review Letters, 94, 170201, 2005.

(32) Jarrell, M.; Tomko, K.; Maier, T.; D'Azevedo, E.; Scalettar, R.; Bai, Z.; Savrasov, S. Next Generation Multi-Scale Quantum Simulation Software for Strongly Correlated Materials. Institute of Physics Publishing, 78, 012031, 2007.

(33) Dedominicis, C.; Martin, P. C. Stationary Entropy Principle + Renormalization in Normal + Superfluid Systems .I. Algebraic Formulation. Journal of Mathematical Physics, 5, 14-30, 1964.

(34) Babu, S.; Brown, G. E. Quasiparticle Interaction in Liquid He-3. Annals of Physics, 78, 1-38, 1973.

(35) Ainsworth, T.; Bedell, K.; Brown, G.; Quader, K. A Model for Paramagnetic Fermi Systems. Journal of Low Temperature Physics, 50, 319-336, 1983.

(36) Quader, K.; Bedell, K.; Brown, G. Strongly Interacting Fermions. Physical Review B, 36, 156-167, 1987.

(37) Pfitzner, M.; Wölfle, P. Quasiparticle Interaction in the Fermi Liquid ^{3}He. Physical Review B, 35, 4699-4712, 1987.

(38) Perdew, J. P.; Staroverov, V. N.; Tao, J. M.; Scuseria, G. E. Density Functional with Full Exact Exchange, Balanced Nonlocality of Correlation, and Constraint Satisfaction. Physical Review A, 78, 052513, 2008.

(39) Kikuchi, Y.; Belosludov, R. V.; Baba, H.; Farajian, A. A.; Mizuseki, H.; Kawazoe, Y. Structure and Electronic Properties of Metal Di-(4-Thiophenyl)-Porphyrin. Taylor & Francis Ltd, 929-933, 2004.

(40) Jasat, A.; Dolphin, D. Expanded Porphyrins and Their Heterologs. Chemical Reviews, 97, 2267-2340, 1997.

(41) Inabe, T.; Tajima, H. Phthalocyanines - Versatile Components of Molecular Conductors. Chemical Reviews, 104, 5503-5533, 2004.

(42) de la Torre, G.; Vaquez, P.; Agullo-Lopez, F.; Torres, T. Role of Structural Factors in the Nonlinear Optical Properties of Phthalocyanines and Related Compounds. Chemical Reviews, 104, 3723-3750, 2004.

(43) Ren, T. Peripheral Covalent Modification of Inorganic and Organometallic Compounds through C-C Bond Formation Reactions. Chemical Reviews, 108, 4185-4207, 2008.

(44) Gatteschi, D.; Sessoli, R.; Cornia, A. Single-Molecule Magnets Based on Iron(III) Oxo Clusters. Chemical Communications, 725-732, 2000.

(45) Jolivet, J. P.; Tronc, E.; Chaneac, C. Iron Oxides: From Molecular Clusters to Solid. A Nice Example of Chemical Versatility. Comptes Rendus Geoscience, 338, 488-497, 2006.

(46) Murugesu, M.; Abboud, K. A.; Christou, G. New Hexanuclear and Dodecanuclear Fe(III) Clusters with Carboxylate and Alkoxide-Based Ligands from Cluster Aggregation Reactions. Polyhedron, 23, 2779-2788, 2004.

(47) Novak, M. A. Magnetic Relaxation in Molecular Nanostructures. Journal of Magnetism and Magnetic Materials, 272, E707-E713, 2004.

(48) Datta, S. Nanoscale Device Simulation: The Green's Function Method. Superlattices and Microstructures, 28, 253-278, 2000.

(49) Damle, P. S.; Ghosh, A. W.; Datta, S. Unified Description of Molecular Conduction: From Molecules to Metallic Wires. Physical Review B, 64, 201403, 2001.

(50) Wagner, M. Expansions of Nonequilibrium Green's Functions. Physical Review B, 44, 6104-6117, 1991.

(51) Rammer, J.; Smith, H. Quantum Field-Theoretical Methods in Transport Theory of Metals. Reviews of Modern Physics, 58, 323-359, 1986.

(52) Barriere, F.; Fabre, B.; Hao, E.; LeJeune, Z. M.; Hwang, E.; Garno, J. C.; Vicente, M. G. H. Electropolymerizable 2,2'-Carboranyldithiophenes. Structure-Property Investigations of the Corresponding Conducting Polymer Films by Electrochemistry, Uv-Visible Spectroscopy and Conducting Probe Atomic Force Microscopy. Macromolecules, in press, 2009.

(53) Hwang, E.; deSilva, K. M. N.; Seevers, C. B.; Li, J.-R.; Garno, J. C.; Nesterov, E. E. Self-Assembled Monolayer Initiated Electropolymerization: A Route to Thin-Film Materials with Enhanced Photovoltaic Performance. Langmuir, 24, 9700-9706, 2008.

(54) Spinu, L.; Pham, H.; Radu, C.; Denardin, J. C.; Dumitru, I.; Knobel, M.; Dorneles, L. S.; Schelp, L. F.; Stancu, A. Probing Two-Dimensional Magnetic Switching in Co/Sio2 Multilayers Using Reversible Susceptibility Experiments. Applied Physics Letters, 86, 012506, 2005.

(55) Spinu, L.; Stancu, A.; Kubota, Y.; Ju, G.; Weller, D. Vectorial Mapping of Exchange Anisotropy in Irmn/Feco Multilayers Using the Reversible Susceptibility Tensor. Physical Review B, 68, 220401(R), 2003.

(56) Kolesnichenko, V. In Magnetic Nanoparticles; Gubin, S. P., Ed.; Wiley-VCH: Verlag, Weinheim, 2009, p 25-58.

(57) Goloverda, G.; Jackson, B.; Kidd, C.; Kolesnichenko, V. Synthesis of the Ultrasmall Nanoparticles of Magnetic Iron Oxides and Study of Their Colloid and Surface Chemistry. Journal of Magnetism and Magnetic Materials, 321, 1372-1376, 2009.

(58) Kimura, T.; Goto, T.; Shintani, H.; Ishizaka, K.; Arima, T.; Tokura, Y. Magnetic Control of Ferroelectric Polarization. Nature, 426, 55-58, 2003.

(59) Chiba, D.; Sawicki, M.; Nishitani, Y.; Nakatani, Y.; Matsukura, F.; Ohno, H. Magnetization Vector Manipulation by Electric Fields. Nature, 455, 515-518, 2008.

(60) Novosad, V.; Otani, Y.; Ohsawa, A.; Kim, S. G.; Fukamichi, K.; Koike, J.; Maruyama, K.; Kitakami, O.; Shimada, Y. Novel Magnetostrictive Memory Device. 6400-6402, 2000.

(61) Nana, C.-W.; Bichurin, M. I.; Dong, S.; Viehland, D.; Srinivasan, G. Multiferroic Magnetoelectric Composites: Historical Perspective, Status, and Future Directions. Journal of Applied Physics, 103, 031101, 2008.

(62) Hur, N.; Park, S.; Sharma, P.; Ahn, J.; Guha, S.; Cheong, S. Electric Polarization Reversal and Memory in a Multiferroic Material Induced by Magnetic Fields. Nature, 429, 392-395, 2004.

(63) Kamihara, Y.; Hiramatsu, H.; Hirano, M.; Kawamura, R.; Yanagi, H.; Kamiya, T.; Hosono, H. Iron-Based Layered Superconductor: Laofep. Journal of the American Chemical Society, 128, 10012-10013, 2006.

(64) Grant, P. M. Superconductivity: Prospecting for an Iron Age. Nature, 453, 1000-1001, 2008.

(65) Mazin, I. I.; Singh, D. J.; Johannes, M. D.; Du, M. H. Unconventional Superconductivity with a Sign Reversal in the Order Parameter of $LaFeAsO_{1-X}F_x$. Physical Review Letters, 101, 057003, 2008.

(66) Sawatzky, G. A.; Elfimov, I. S.; van der Brink, J.; Zaanen, J. Heavy-Anion Solvation of Polarity Fluctuations in Pnictides. Europhysics Letters, 86, 17006, 2009.

(67) Broun, D. M. What Lies beneath the Dome? Nature Physics, 4, 170-172, 2008.

(68) Vidhyadhiraja, N. S.; Macridin, A.; Sen, C.; Jarrell, M.; Ma, M. Quantum Critical Point at Finite Doping in the 2d Hubbard Model: A Dynamical Cluster Quantum Monte Carlo Study. Physical Review Letters, 102, 206407, 2009.

(69) Yang, L.; Fishbine, B. K.; Migliori, A.; Pratt, L. R. Molecular Simulation of Electrochemical Capacitors Based on Nanotube Forests. Journal of the American Chemical Society, 131, 12373-12376, 2009.

(70) Nellas, R. B.; Keasler, S. J.; Chen, B. Molecular Content and Structure of Aqueous Organic Nanodroplets from the Vapor-Liquid Nucleation Study of the Water/N-Nonane/1-Alcohol Series. The Journal of Physical Chemistry A, 112, 2930-2939, 2008.

(71) Nellas, R.; McKenzie, M.; Chen, B. Probing the Nucleation Mechanism for the Binary N-Nonane/1-Alcohol Series with Atomistic Simulations. Journal of Physical Chemistry B, 110, 18619-18628, 2006.

(72) Nellas, R.; Chen, B.; Siepmann, J. Dumbbells and Onions in Ternary Nucleation. Physical Chemistry Chemical Physics, 9, 2779-2781, 2007.

(73) Nellas, R.; Chen, B. Towards Understanding the Nucleation Mechanism for Multi-Component Systems: An Atomistic Simulation of the Ternary Nucleation of Water/N-Nonane/1-Butanol. Physical Chemistry Chemical Physics, 10, 506-514, 2008.

(74) Kathmann, S.; Schenter, G.; Garrett, B.; Chen, B.; Siepmann, J. Thermodynamics and Kinetics of Nanoclusters Controlling Gas-to-Particle Nucleation. The Journal of Physical Chemistry C, 113, 10354-10370.

(75) Chen, B.; Siepmann, J. I.; Klein, M. L. Simulating Vapor-Liquid Nucleation of Water: A Combined Histogram-Reweighting and Aggregation-Volume-Bias Monte Carlo Investigation for Fixed-Charge and Polarizable Models. Journal of Physical Chemistry A, 109, 1137-1145, 2005.

(76) Panagiotopoulos, A. Z. Direct Determination of Phase Coexistence Properties of Fluids by Monte-Carlo Simulation in a New Ensemble. Molecular Physics, 61, 813-826, 1987.

(77) Panagiotopoulos, A. Z. Direct Determination of Fluid-Phase Equilibria by Simulation in the Gibbs Ensemble - a Review. Molecular Simulation, 9, 1-23, 1992.

(78) Smit, B.; Desmedt, P.; Frenkel, D. Computer-Simulations in the Gibbs Ensemble. Molecular Physics, 68, 931-950, 1989.

(79) Escobedo, F. A.; Depablo, J. J. Monte-Carlo Simulation of the Chemical-Potential of Polymers in an Expanded Ensemble. Journal of Chemical Physics, 103, 2703-2710, 1995.

(80) Lyubartsev, A. P.; Martsinovski, A. A.; Shevkunov, S. V.; Vorontsovvelyaminov, P. N. New Approach to Monte-Carlo Calculation of the Free-Energy - Method of Expanded Ensembles. Journal of Chemical Physics, 96, 1776-1783, 1992.

(81) Yu, B.; Browne, D.; Kleban, P. Monte Carlo Study of Co Oxidation on an Anisotropic Surface. Physical Review A, 43, 1770-1776, 1986.

(82) Aukrust, T.; Browne, D. A.; Webman, I. Critical-Behavior of an Autocatalytic Reaction Model. Physical Review A, 41, 5294-5301, 1990.

(83) Aukrust, T.; Browne, D. A.; Webman, I. Kinetic Phase-Transition in a One-Component Irreversible Reaction Model. Europhysics Letters, 10, 249-255, 1989.

(84) Bustamante, F.; Enick, R. M.; Killmeyer, R. P.; Howard, B. H.; Rothenberger, K. S.; Cugini, A. V.; Morreale, B. D.; Ciocco, M. V. Uncatalyzed and Wall-Catalyzed Forward Water-Gas Shift Reaction Kinetics. American Institute of Chemical Engineers, Journal, 51, 1440-1454, 2005.

(85) Seetala, N. V.; Bass, J.; Jayasingha, A. M. R.; Garudadri, R. K.; Siriwardane, U. Sol-Gel Prepared Cu-Ce-Ni Nanoparticle Alumina Catalysts for Wgs Hydrogen Production. Microscopy and Microanalysis, 14, 308-309, 2008.

(86) Wilson, C.; Brown, J.; McDonald, J. M., US Patent pending

(87) Lomnicki, S.; Truong, H.; Vejerano, E.; Dellinger, B. Copper Oxide-Based Model of Persistent Free Radical Formation on Combustion-Derived Particulate Matter. Environmental Science & Technology, 42, 4982-4988, 2008.

(88) McFerrin, C. A.; Hall, R. W.; Dellinger, B. Ab Initio Study of the Formation and Degradation Reactions of Chlorinated Phenols. Journal of Molecular Structure-Theochem, 902, 5-14, 2009.

(89) Bae, G.-T.; Hall, R. W. In Preparation, 2009. Density functional calculation of the structure and electronic properties of Cu_n O_n (n=1-7) clusters.

(90) Dutta, R. C. Drug Carriers in Pharmaceutical Design: Promises and Progress. Current Pharmaceutical Design, 13, 761-769, 2007.

(91) Vicent, M. J.; Duncan, R. Polymer Conjugates: Nanosized Medicines for Treating Cancer. Trends in Biotechnology, 24, 39-47, 2006.

(92) MacKerell, A. D.; Wiorkiewicz-Kuczera, J.; Karplus, M. An All-Atom Empirical Energy Function for the Simulation of Nucleic Acids Journal of the American Chemical Society, 117, 11946-11975, 1995.

(93) Brooks, B. R.; Bruccoleri, R. E.; Olafson, B. D.; States, D. J.; Swaminathan, S.; Karplus, M. CHARMM - a Program for Macromolecular Energy, Minimization, and Dynamics Calculations Journal of Computational Chemistry, 4, 187-217, 1983.

(94) Cornell, W. D.; Cieplak, P.; Bayly, C. I.; Gould, I. R.; Merz, K. M.; Ferguson, D. M.; Spellmeyer, D. C.; Fox, T.; Caldwell, J. W.; P.A. Kollman. A 2nd Generation Force-Field for the Simulation of Proteins, Nucleic Acids, and Organic Molecules. Journal of the American Chemical Society, 117, 5179-5197, 1995.

(95) Oostenbrink, C.; Villa, A.; Mark, A. E.; Gunsteren, W. F. v. A Biomolecular Force Field Based on the Free Enthalpy of Hydration and Solvation: The GROMOS Force-Field Parameter Sets 53a5 and 53a6 Journal of Computational Chemistry, 25, 1656-1676, 2004.

(96) Gunsteren, W. F. v.; Billeter, S. R.; Eising, A. A.; Hunenberger, P. H.; Kruger, P.; Mark, A. E.; Scott, W. R. P.; Tironi, I. G. Biomolecular Simulations: The GROMOS96 Manual and User Guide, vdf Hochschulverlag AG an der ETH Zurich, Zurich1996.

(97) Jorgensen, W. L.; Maxwell, D. S.; Tirado-Rives, J. Development and Testing of the OPLS All-Atom Force Field on Conformational Energetics and Properties of Organic Liquids. Journal of the American Chemical Society, 118, 11225-11236, 1996.

(98) Marrink, S. J.; Risselada, H. J.; Yefimov, S.; Tieleman, D. P.; Vries, A. H. d. The MARTINI Force Field: Coarse Grained Model for Biomolecular Simulations. Journal of Physical Chemistry B, 111, 7812-7824, 2007.

(99) Monticelli, L.; Kandasamy, S. K.; Periole, X.; Larson, R. G.; Tieleman, D. P.; Marrink, S.-J. The MARTINI Coarse-Grained Force Field: Extension to Proteins Journal of Chemical Theory and Computation, 4, 819-834, 2008.

(100) Kolb, H.; Finn, M.; Sharpless, K. Click Chemistry: Diverse Chemical Function from a Few Good Reactions. Angewandte Chemie International Edition, 40, 2004-2021, 2001.

(101) Tornoe, C.; Christensen, C.; Meldal, M. Peptidotriazoles on Solid Phase:[1, 2, 3]-Triazoles by Regiospecific Copper (I)-Catalyzed 1, 3-Dipolar Cycloadditions of Terminal Alkynes to Azides. Journal of Organic Chemistry, 67, 3057-3064, 2002.

(102) Helms, B.; Mynar, J.; Hawker, C.; Frechet, J. Dendronized Linear Polymers Via "Click Chemistry". Journal of the American Chemical Society, 126, 15020-15021, 2004.

(103) Malkoch, M.; Schleicher, K.; Drockenmuller, E.; Hawker, C.; Russell, T.; Wu, P.; Fokin, V. Structurally Diverse Dendritic Libraries: A Highly Efficient Functionalization Approach Using Click Chemistry. Macromolecules, 38, 3663-3678, 2005.

(104) Laurent, B.; Grayson, S. An Efficient Route to Well-Defined Macrocyclic Polymers Via "Click" Cyclization. Journal of the American Chemical Society, 128, 4238-4239, 2006.

(105) Liu, S.; Gibb, B. High-Definition Self-Assemblies Driven by the Hydrophobic Effect: Synthesis and Properties of a Supramolecular Nanocapsule. Chemical Communications, 2008, 3709-3716, 2008.

(106) Laurent, B.; Grayson, S. Synthesis of Linear and Cyclic Amphiphilic Homopolymers as Unimolecular Invertible Micelles. Polymeric Materials Science and Engineering, 98, 502-503, 2008.

(107) Gao, H.; Matyjaszewski, K. Synthesis of Molecular Brushes by "Grafting onto" Method: Combination of Atrp and Click Reactions. Journal of the American Chemical Society, 129, 6633-6639, 2007.

(108) Li, Y.; Giles, M.; Grayson, S. Assembly of Star Polymers by Clicking Linear Polymers to Poly(Alkynated) Dendrimers. Polymeric Materials Science and Engineering, 98, 509-510, 2008.

(109) Ashbaugh, H.; Patel, H.; Kumar, S.; Garde, S. Mesoscale Model of Polymer Melt Structure: Self-Consistent Mapping of Molecular Correlations to Coarse-Grained Potentials. The Journal of chemical physics, 122, 104908, 2005.

(110) Price, R. R.; Gaber, B. P.; Lvov, Y. In-Vitro Release Characteristics of Tetracycline HCl, Khellin and Nicotinamide Adenine Dineculeotide from Halloysite; a Cylindrical Mineral. Journal of Microencapsulation, 18, 713-722, 2001

(111) Lvov, Y.; Shchukin, D.; Möhwald, H.; Price, R. Halloysite Clay Nanotubes for Controlled Release of Protective Agents. ACS nano, 2, 814-820, 2008.

(112) Derosa, P.; Kolan, B.; Gold, S. Proton Diffusion in Nanopores, MD Simulation. Proceedings of the American Institute of Chemical Engineering. 2007.

(113) Hess, B.; Kutzner, C.; van der Spoel, D.; Lindahl, E. GROMACS 4: Algorithms for Highly Efficient, Load-Balanced, and Scalable Molecular Simulation. Journal of Chemical Theory and Computation, 4, 435-447, 2008.

(114) Plimpton, S. J. Fast Parallel Algorithm for Short-Range Molecular Dynamics. Journal of Computational Physics, 117, 1-19, 1995.

(115) Soppimath, K. S. L., L. H.; Seow, W. Y.; Liu, S. Q.; Powell, R.; Chan, P.; Yang, Y. Y. Multifunctional Core/Shell Nanoparticles Self-Assembled from Ph-Induced Thermosensitive Polymers for Targeted Intracellular Anticancer Drug Delivery. Advanced Functional Materials, 17, 355-362, 2007.

(116) http://www.theinstitute.smu.edu/parity_about.html, last access date: July 25, 2009

(117) Collins, S. N.; Stanley, G. G.; Warner, I. M.; Watkins, S. F. What Is Louisiana State Doing Right? Chemical and Engineering News, 79, 39-42, 2001.

(118) http://www.laworks.net/Downloads/Employment/AffirmativeActionPublication_2008.pdf, last access date: July 10, 2009

(119) http://www.cct.lsu.edu/BeowulfSummerCamp, last access date: July 25, 2009

(120) Exploring the Concept of Undergraduate Research Centers: A Report on the NSF Workshop, National Science Foundation, Division of Chemistry, Office of Special Projects, Office of Multidisciplinary Activities, MPS Directorate, 2003.

(121) http://sc09.sc-education.org, last access date: July 25, 2009

(122) https://www.msu.edu/~first4/, last access date: June 9, 2009

(123) Alexeev, Y.; Allan, B.; Armstrong, R.; Bernholdt, D.; Dahlgren, T.; Gannon, D.; Janssen, C.; Kenny, J.; Krishnan, M.; Kohl, J. Component-Based Software for High-Performance Scientific Computing, Institute of Physics Publishing, Vol, 16, 2005.

(124) Thomas, M.; Burruss, J.; Cinquini, L.; Fox, G.; Gannon, D.; Gilbert, L.; von Laszewski, G.; Jackson, K.; MIddleton, D.; Moore, R. Grid Portal Architectures for Scientific Applications, Institute for Physics Publishing, Vol, 16, 2005.