



## Materials Science Alliance Awarded Largest NSF Grant in Louisiana

Louisiana EPSCoR has been awarded a \$20 million Research Infrastructure Improvement (RII) grant that represents the largest ever awarded to Louisiana by NSF.

Louisiana plans to transform materials science research of modern materials that drive today's technologies by creating the Louisiana Alliance for Simulation-Guided Materials Applications (LA-SiGMA). This research will study the complex behavior of materials related to everything from biomolecular systems and drug delivery to energy storage.

A major research focus of LA-SiGMA 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: correlated electronic materials, energy materials and biomolecular materials.

Research outcomes include: Statewide research and education programs in materials science; Strong multidisciplinary and multi-institutional research teams; Multiscale simulation tools for 21<sup>st</sup> century computing environments; A National Center of Excellence in simulation-guided materials applications.

### Correlated electronic materials

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

magnets and organic semiconductors.

### Energy materials

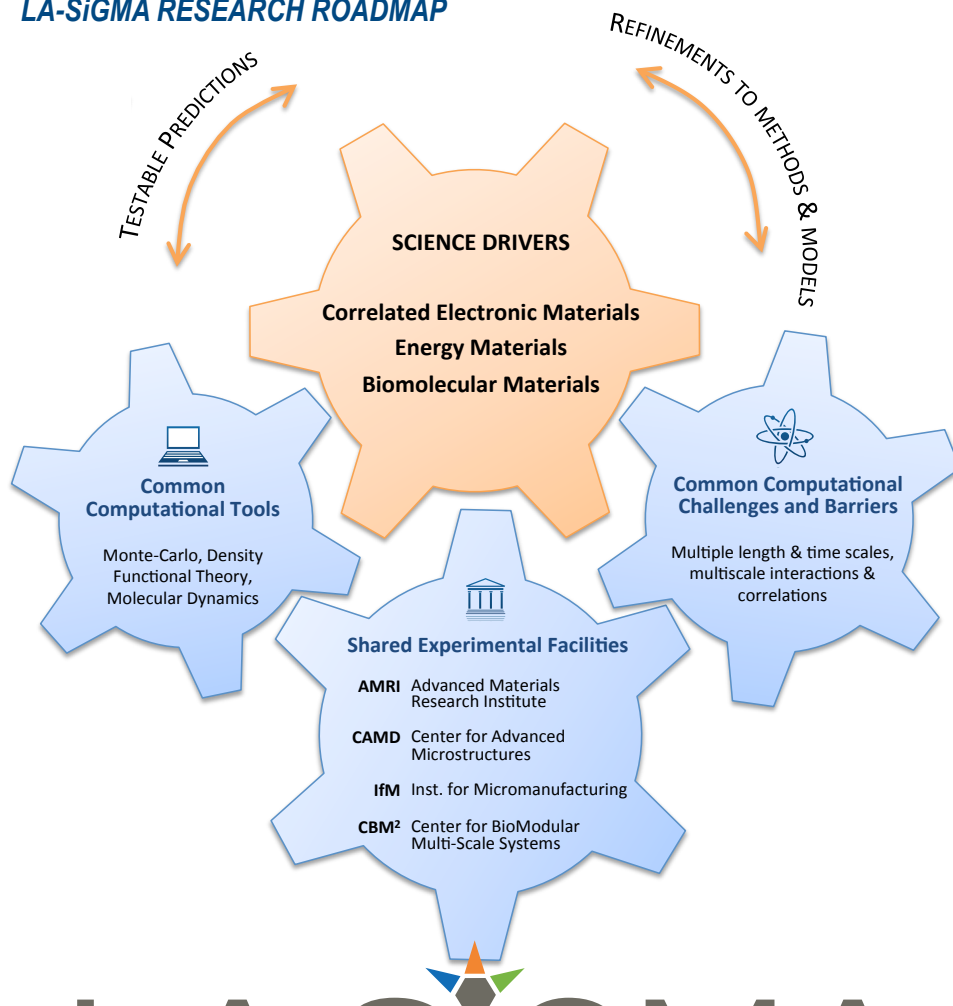
The energy materials science driver will focus on the use of novel simulation methods to overcome the multiple time scales barriers in electrical storage materials, hydrogen fuels and catalytic reactions involving metal oxides. The resulting

research will help the design of better electrochemical capacitors, fuel cells, hydrogen storage materials and metal oxide catalysts.

### Biomolecular materials

The goal of the biomolecular science driver is to develop novel biomolecular material systems, such as halloysite nanotubes, for the encapsulation,

### LA-SiGMA RESEARCH ROADMAP



# LA-SiGMA

Louisiana Alliance for Simulation-Guided Materials Applications

delivery, and release of therapeutics to targeted tissues.

The commonality of the computational tools is the “glue” that tightly integrates the three science drivers.

LA-SiGMA's multi-institutional collaborations will leverage new cutting edge computational tools and experimental methods as information technology continues to rapidly transform in scope and power.

The project will not only have broad scientific significance, it will also dramatically impact education and workforce development in the State by creating a comprehensive set of programs addressing various demographic needs.

One approach will be a comprehensive workforce development plan involving high school, two-year college, and undergraduation students in research.

Training will be offered to teachers that focuses on teaching methods for computational materials science. In addition, two-year college students will be able to take training courses in the use of state-of-the-art laboratory instrumentation and high-performance computing systems.

At the same time, initiatives are planned to increase the participation of women and underrepresented groups in LA-SiGMA activities as well

as recruit outstanding faculty into Alliance institutions.

LA-SiGMA will include more than 100 faculty, postdoctoral researchers and students from seven universities and will be sustained by collaborations involving shared students and postdoctoral researchers, interdisciplinary programs in computational materials, and shared courses taught via HD video.

The LA-SiGMA Alliance collaborating members include: Louisiana State University, Grambling State University, Louisiana Tech University, Southern University at Baton Rouge, Tulane University, University of New Orleans, and Xavier University of Louisiana.

“The formation of LA-SiGMA through the support of this NSF EPSCoR grant will enable Louisiana to position itself to transform research and education in computational materials science, a relatively young field,” says Dr. Michael Khonsari, project director of Louisiana's EPSCoR program and Associate Commissioner for Sponsored Programs at the Louisiana Board of Regents.

The award includes a state investment of \$10 million, through the Board of Regents Support Fund and over \$3.5 million from participating institutions.

The Support Fund, which has

“This NSF award represents a big win for our state as it will directly assist with the development of several of our Blue Ocean target industries including renewable energy, pharmaceuticals, next-wave oil and gas, next-generation automotive manufacturing and nuclear energy components manufacturing.”

- Stephen Moret,  
Secretary, Louisiana  
Economic Development

provided matching monies since inception of the LA EPSCoR program, is a crucial partner in securing federal funding, providing important resources to undergird the work and tangibly demonstrating the State's commitment to the projects.

“The combination of NSF EPSCoR and Support Fund dollars has been essential to attracting a growing stream of federal funding and private-sector investment in projects which faculty have generated,” said Kerry Davidson, Deputy Commissioner for Sponsored Programs. “This has contributed significantly to building and sustaining 21st-century research efforts across the State.”