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CCT's Material World focus area to enhance advanced materials research at LSU

New-generation batteries, faster computer chips, more effective medication, synthetic fibers in bullet-proof clothing, substitutes for critical minerals, packaging that would keep food fresh longer–advanced materials are a part of our everyday lives. The interdisciplinary nature of Louisiana State University's Center for Computation & Technology, or CCT, makes it an ideal setting for LSU scientists to conduct advanced materials research.

CCT's Material World focus area unites faculty from many departments who focus on novel approaches in materials science. Unlike the traditional model, "given the material, find the property," the new approach is "given the property, find the material."

"We are developing materials with greater functionality," said Mark Jarrell, Material World focus area lead and a professor at LSU's Department of Physics & Astronomy. "To design materials with specific functions, we need to accurately describe the physics and chemistry that's at work," he said. "Our–high speed computing and high-speed networks–are becoming more robust, which helps narrow the design space."

One example of the phenomena the Material World focus area explores is superconductivity. It happens when a substance, typically metallic or ceramic, reaches its critical temperature and loses all electrical resistance. This occurs at extremely low temperatures, which makes it difficult to apply to real-life situations.

Collaborating with Mark Jarrell, Juana Moreno, faculty member in CCT's Material World focus area and an associate professor in LSU's Department of Physics & Astronomy, is trying to understand how to develop superconductive materials that would work at room temperature. These materials transport energy very efficiently, and have great potential for applications in electronic devices, transportation, and also power transmission, generation, and storage.

"Computational materials is a very integrated effort in Louisiana," Moreno said. "We are part of the Louisiana Alliance for Simulation-Guided Materials Applications, or LA-SiGMA, that creates a statewide research and education program focusing on three science drivers: electronic, energy, and biomolecular materials."

Created in 2010, the LA-SiGMA initiative became one of the largest National Science Foundation grants that Louisiana had ever received —$20 million.

In 2013, four new LSU faculty joined CCT's Material World focus area, because they recognized that it offers a unique environment in which to nurture their research.

Among them is Bill Shelton, a nationally prominent materials scientist who was hired jointly by the Department of Chemical Engineering. His research area involves advanced materials used in the auto, aerospace, military, and electronics industry.

"Light-weight and high-strength alloy systems are important for applications in the auto industry to lighten the vehicle for better fuel efficiency while maintaining safety," Shelton said. "Another type of materials—light-weight, high-strength, and high-temperature materials —is used in turbine blades for improved fuel efficiency of an airplane as they allow for running the turbine engines at higher temperatures. What's more, these high-strength materials are used for military applications to withstand armaments," he said.

Another CCT's new hire, Revati Kumar, who also joined LSU's chemistry department this fall, forms a molecular level understanding of electrolyte behavior in rechargeable batteries. Electrolyte is the material that separates anode and cathode, and through which ions are transported. Its degradation can significantly reduce the battery's life.

"To design the next generation of batteries, it is imperative that we understand the factors that reduce their life cycle. My research focuses on electrolyte optimization–an important component of battery systems," Kumar said.

Kenneth Lopata joined LSU's chemistry department and CCT this fall, too. He studies electrons and nuclei in motion.

"When light hits matter, it causes electrons, and in turn nuclei, to move, resulting in millionth of a billionth of a second changes in the material," Lopata said. "This extremely fast motion is crucial in materials such as photovoltaics, for example, where light is absorbed by a material and converted to electrical energy," he said.

Advanced materials research not only deals with metals, crystals and liquids, but can also involve biological systems. CCT's Michal Brylinski, who has a joint appointment with LSU's Department of Biological Sciences, models strings of protein molecules, putting them together in different configurations. This helps him understand how a certain bacteria or a drug connects to the surface of a cell and interacts with it at the atomic level.

"Studying a protein in isolation is not enough, because it interacts with other proteins that could modify its function, so I have to put each protein in a context of a living cell," Brylinski said.

Yet another area where advanced materials research can be applied is Earth science. Jianwei Wang, who joined LSU's Department of Geology & Geophysics and CCT's Material World group this fall, does just that.

"I do molecular modeling to understand properties of geomaterials," Wang said. "The results are used to predict material properties in geological processes. For example, by linking interactions of contaminants (natural or man-made) with rocks in underground water systems to their molecular scale controls at mineral-water interfaces, the transport of the contaminants can be better predicted and the environmental impact can be addressed a priori," Wang said.

"All CCT's materials scientists share the need for taking a certain set of mathematical equations and teaching the supercomputer to solve them effectively. The techniques that they use overlap, and this is why they benefit so much from interacting with one another," said CCT's Director Joel Tohline.

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