

University of Minnesota receives \$13.1 million in Department of Energy funding for two new nationwide centers

Centers will include research on CO2 capture and solar energy conversion

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MINNEAPOLIS / ST. PAUL (08/22/2012) —The University of Minnesota has been awarded two grants from the U.S. Department of Energy (DOE) totaling \$13.1 million over the next five years to fund two nationwide centers headquartered in the Department of Chemistry in the University's College of Science and Engineering.

Research within the two centers will include developing new materials related to capturing greenhouse gases and improving chemical processes as well as developing methods and software tools for increasing the efficiency of solar energy conversion. Both centers will begin research activities Sept. 1, 2012.

Both of these grants were very competitive with many other institutions submitting proposals and only a handful chosen for each, said University of Minnesota chemistry professors Laura Gagliardi and Christopher J. Cramer, who will lead the University's two new centers. "It's very rare to have two major DOE initiatives at the same institution, but the proposal reviews indicate that we were chosen because of our excellent researchers and the University's Minnesota Supercomputing Institute, which provides state-of-the-art computing facilities," Gagliardi said.

The **Nanoporous Materials Genome Center** will be funded with \$8.1 million over five years as a DOE Center for Materials or Chemical Science Software Innovation. The center will develop and use high-end computational tools to characterize and predict the performance of millions of advanced materials at the nano scale. These new materials have many potential applications related to energy, including the capture of greenhouse gases, such as CO₂, and the storage of hydrogen. In addition, the group aims to improve catalysis and advanced chemical separations used in environmental research, as well those used in petroleum and biofuels processes to make them more efficient and environment-friendly.

The Nanoporous Materials Genome Center will be based at the University of Minnesota and include researchers from six other institutions including the University of California, Berkeley; Lawrence Berkeley National Laboratory; Washington State University; Rice University; Georgia Tech; and Northwestern University. University of Minnesota chemistry professor Laura Gagliardi will serve as the center's director.

"It's wonderful opportunity for us to collaborate with our colleagues nationwide to make significant contributions in important areas of environmental research," Gagliardi said.

The **Center for the Study of Charge Transfer and Charge Transport in Photoactivated Systems** is funded by a \$5 million grant over five years through the DOE Scientific Discovery through Advanced Computing (SciDAC) initiative. Researchers will develop methods, algorithms, and improve software tools needed for the reliable modeling of charge transfer and charge transport in photoactivated systems. Such processes are fundamental for solar energy capture, solar energy conversion, and photoactivated catalysis, both industrial and biological. University of Minnesota

chemistry professor Christopher J. Cramer will serve as center director.

Research partners include: Pacific Northwest National Laboratory and Lawrence Berkeley National Laboratory.

“The computational chemistry group here at the University of Minnesota is world-class, with an outstanding record of accomplishments,” said William B. Tolman, chair of the University of Minnesota Department of Chemistry. “Their expertise in theory development and applications is second to none, putting them in a great position to make significant research progress on the critical problems targeted by the DOE center grant proposals.”

In addition to Gagliardi and Cramer, other participating University of Minnesota faculty involved in the centers include chemistry professors Donald G. Truhlar and J. Ilja Siepmann and chemical engineering and materials science professor Michael Tsapatsis.

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Last modified on August 22, 2012