Introduction to Completed Project Reports

Solar

Professors Zhenan Bao, Michael Toney, and Alan Aspuru-Guzik began a project in 2010 aimed toward breakthrough performance solar cells by rational organic semiconductor material design. This project combined the molecular design and device fabrication expertise of Bao, theoretical simulation expertise of Aspuru-Guzik, and the structural characterization expertise of Toney. The large distributed computing power of IBM's World Community Grid (WCG) allowed the rational design of organic semiconductors for solar cells from a new angle. Many achievements have been made including the development of high efficiency and polymer/polymer solar cells, the precise molecular packing structures for thin films of pentacene, and TIPSE-pentacene. A series of fluorine-bithiophene oligomers from grazing incidence X-ray diffraction (GIXD) data combined with numerical fitting has been determined. In the last year the molecular library of the candidate compounds has been expanded and the infrastructure underlying the Clean Energy Project improved. The computational high-throughput screening of candidate structures is increasingly becoming a powerful tool in the search for novel organic electronic materials and is gathering interest in the community.

Biomass

In the area of lignin management, one program has ended within the last year by Professors Claire Halpin and Gordon Simpson at the University of Dundee. Their project was aimed at identifying and studying novel mutants optimized for lignin, growth and biofuel production via re-mutagenesis. Their work involved the use of a saccharification screen to identify mutants in the model plant Arabidopsis thaliana that are more easily processed to biofuels and determining the underlying genetics of these to enable transfer of knowledge to biofuels crops. Exciting findings from both Halpin and Boerjan's research prompted the request for a patent filing on a gene family that when knocked out in plants has a marked increase in the sugar release from the plants under mild processing conditions. This finding led to a publication that made the cover of *Science*. Additional interesting mutants and genes were found during this study and these will likely lead to further publications in the near future.

Grid Storage

Professor Robert Hebner at the University of Texas, Austin and Professor Ray Baughman at the University of Texas, Dallas, concluded research efforts on "A Low-Cost Flywheel Design and Flywheel Materials". The group at UT Dallas has been working with CNT fibers and composites to create multifunctional materials that combine high strength with the magnetic and superconducting properties needed to levitate rotors for flywheel batteries. The UT Austin group designed codes and methods for incorporating the materials into the flywheel bearing designs. Promising results show that flywheel storage may have potential applications for diurnal energy storage. In this past year, UT-CEM used their design code and material results from UT Dallas to study the potential impact of these advanced technologies for flywheel energy storage. These results showed that significant improvements could be made to energy storage density utilizing magnetically filled nano-composites in the flywheel bearing design.