Introduction to Completed Project Reports

Hydrogen

Professor Swartz and his team have been working towards a cost-effective technology for the production of hydrogen from glucose, xylose, and other by products of cellulosic biomass. Initial work demonstrated feasibility of using an unpurified cell extract to enable glucose conversion into hydrogen as well as further improvement of hydrogen production through screening of naturally occurring ferredoxin NADP+ reductases and ferredoxins and use of fusion proteins. Recently the focus has been on engineering these proteins to further improve productivity in the synthetic pathway as well as engineering the cell extract to improve yield. They have established the platform for cell free metabolic conversion of glucose to hydrogen as well as the previously described selective metabolic silencing (SeMS) technology. While there is still much work to do in order to reach industrial feasibility, the researchers have been able to make significant gains in both rate of hydrogen production (>15X) and the overall yield of a cell free process coupled with a synthetic pathway. All of this work together continues to establish an alternative method for sustainable biochemical production using low cost feedstocks and cell free extracts coupled with synthetic biology. This work so far has led to a patent application.

Solar

Professors Mike McGehee and Alan Sellinger of Stanford University, and Colorado School of Mines respectively, began a project in 2010 aimed at investigating advanced electron transport materials for application in organic photovoltaics (OPVs). The objectives of the proposed work are to design, prepare and characterize a family of new advanced electron transport materials from simple, minimal step, high yield, and inexpensive synthetic processes for application in OPVs. In the past year, significant progress in the discovery of the mechanisms underlying how devices prepared with new electron acceptor materials generate free charges that contribute to photocurrent has been made. One of the successes of this project is that Sigma-Aldrich became very interested in one of the materials leading to their licensing of the patent and selling under the name PI-BT, product number 790893. The highest efficiency solution-processed bulk heterojunction solar cells prepared without the use of fullerene derivatives have utilized one particular material, 4,7-bis(4-(N-hexylphthalimide) vinyl)benzo[c]1,2,5-thiadiazole, termed HPI-BT. With further improvements in the synthetic preparation of the material and processing conditions, device efficiencies as high as 3.7%, have been achieved. This may be one of the highest efficiencies for solution processed organic solar cells that do not contain fullerene derivatives. Preliminary device lifetime testing results show that OPVs using the HPI-BT electron acceptor are quite long, and this aspect will be looked at further.

Professor Bao's project focused on taking advantage of the potential of carbon-based materials to form an all-carbon solar cell. The different arrangements and combinations in which carbon can exist produce a wide variety of compounds that have unique physical, chemical and electrical properties. Some of these allotropes behave as conductors while others are classified as semiconducting. The efforts of Bao's group focused on taking advantage of the carbon-based materials' potential and optimally we employed them together to form an all carbon solar cell. The final report is divided into the three major directions: sorting strategies of semiconducting single-walled carbon nanotubes for the active solar cell light absorbing materials; doping strategies of carbon-based electrodes; and the demonstration of carbon-based solar cells. Single-walled carbon nanotubes originally come as a mix of metallic and semiconducting tubes; Bao's group developed sorting strategies to specifically select the semiconducting tubes optimal as sensitizers in a solar cell junction. They also developed effective doping strategies of graphene and carbon nanotube based electrodes enabling high conductivity and transparency. All of these separate parts were successfully integrated together in an all-carbon based solar cell.

Professors Jennifer Dionne and Alberto Salleo worked on upconverting electrodes for improved solar energy conversion. Using a suite of analytic calculations, electrodynamic simulations, and state-of-the-art experimental techniques, this project has: predicted the expected photovoltaic efficiency improvements with realistic upconverters; improved existing upconversion processes by precisely controlling photonic and electronic processes; and developed cost-effective upconverting electrodes that can convert near-infrared light to visible light and extract current from solar cells. The innovation in upconverter materials design has yielded record-efficiency upconverting layers, though the efficiencies of these films are still too small for commercial solar applications. Ongoing work is aimed at boosting nearinfrared to visible upconversion efficiencies beyond 10%, and subsequently incorporating these materials into research and commercial solar cells.

Biomass

Professor Alfred Spormann of Stanford University and his group have completed a project on the "Synthesis of biofuels on bioelectrodes". Microbial electrosynthesis of multi-carbon organic compounds is a promising novel technology for converting electricity into renewable organic molecules as well as for storing electrical energy. This project explored the breadth of possible platform organisms to be used in this emerging technology and identified the potential as well as the limitations. Of the multiple microorganism and experimental settings tested, microbial electromethanogenesis is emerging as a strong technology platform, and this work has provided the first insights in the molecular mechanism of cathodic electron uptake as well as operation and resilience of the system. This project has provided the basis for important follow-up studies on microbial electrosynthesis.

CO_2 Storage

Professors Gary Mavko of Stanford University and Andreas Luttge of Rice University led a research effort on "Linking Chemical and Physical Effects of CO_2 Injection to Geophysical Parameters". This project has demonstrated techniques for quantitatively predicting the combined seismic signatures of CO_2 saturation, chemical changes to the rock frame, and pore pressure. This work provided a better understanding of the reaction kinetics of CO_2-bearing reactive fluids with rock-forming minerals. How the resulting long-term CO_2-injection-induced changes to the rock pore space and frame affect seismic parameters in the reservoir was quantified. This research involved laboratory, theoretical, and computational tasks in the fields of both Rock Physics and Geochemistry. Ultrasonic P- and S-wave velocities were measured over a range of confining pressures while injecting CO_2 and brine into the samples. Pore fluid pressure was varied and monitored together with porosity during injection. The measurement of rock physics properties was integrated and complemented by those obtained via geochemical experiments to link the physical and chemical processes underlying the mechanisms triggered by CO_2 injection. The final report summarizes the results of laboratory observations and theoretical, and numerical rock physics models to quantify the P- and S-wave velocities and wave attenuation in partially saturated rocks.

Advanced Combustion

Professor Chris Edwards led a project on “Use of mixed combustion/electrochemical energy conversion to achieve efficiencies in excess of 70% for transportation-scale engines”. The goal of this research is to design an energy conversion system capable of realizing high efficiencies at a smaller scale suitable for distributed generation and transportation. The design for such an engine system is guided by exergy analysis. Past work in the Edward’s lab has shown that in order to achieve ultra high efficiencies, it is necessary to reduce the exergy lost to combustion. The researchers address this loss by utilizing a fuel cell to complement an internal combustion engine in a combined-cycle system that realizes high efficiency. Modeling results of the high-temperature approach indicate an exergy efficiency of 63% (65% LHV) and the team are working to manage operating parameters and device integration to increase this number further. The proposed system includes using devices in unconventional operating regimes, and development of experimental capabilities to validate the models where there is uncertainty in device performance.

Advanced Electric Infrastructure

The project in advanced electric infrastructure is a multi-institutional effort that examines a system-wide effort in the control of the electric network to allow over 50% penetration of renewable energy. This team is led by Professor Kevin Tomsovic at the University of Tennessee, Knoxville and includes three other institutions, University of Illinois, Northeastern University/Tufts University and Rensselaer Polytechnic Institute. The researchers are addressing the five issues surrounding command and control of the electric grid: flat control and communication framework, intelligent device interfaces, optimization with multi-scale energy sources and demands, transmission grid management and operation and test and verification. Most of the institutions aside from Northeastern University/Tufts University have completed their funding period. This is the last report from this project. The analyses suggests that networked estimation/control could be a viable approach to remedy some of the deficiencies in information processing and control for existing electrical power systems, integrating sensing, state/parameter estimation and control to facilitate effective (high-level) control of energy flow. The researchers envision increased couplings among dynamic components in several frequency ranges, which will in turn necessitate development of new coordinated control algorithms, possibly aided by formal verification methods.

Grid Storage

Professors Yi Cui and Robert Huggins at Stanford University were developing inexpensive, safe, high power batteries using aqueous electrolytes. During this GCEP supported project the team have developed a deep scientific understanding of the outstanding electrochemical properties of Prussian Blue Analogue (PBA) materials and their application for grid-scale energy storage and other related technologies. They pursued a number of different research directions, including: cathode and anode materials for grid-scale aqueous batteries, performance of PBAs in organic electrolyte batteries, and insertion of multivalent ions in PBAs for promoting future development of multivalent-ion batteries. They have been highly successful across all of these areas, but notably they developed sodium manganese hexacyanomanganate ($Na_2Mn(II)[Mn(II)(CN)_6]$), an open framework crystal structure material, and found it to be a viable positive electrode for sodium-ion batteries. They have demonstrated a high discharge capacity of 209 mAh g^{-1} at C/5 (40 mA g^{-1}) and excellent capacity retention at high rates in a propylene carbonate electrolyte. These results represent a major step forward in the development of sodium-ion batteries. They also found that nanomaterials in the Prussian Blue family of open framework materials, such as nickel hexacyanoferrate, allow for the reversible insertion of aqueous alkaline earth divalent ions, including Mg^{2+}, Ca^{2+}, Sr^{2+}, and Ba^{2+}. They showed unprecedented long cycle life and high rate performance for divalent ion insertion.