Introduction to Completed Project Reports

Seven GCEP research programs have reached completion during the past year in four portfolio areas of Renewable Energy-Solar, Advanced Coal, Advanced Materials and Catalysts, and Advanced Transportation.

In the area of solar energy, three programs were completed this year. Professors Nate Lewis, Harry Gray, and Harry Atwater of the California Institute of Technology completed a program on the photoelectrochemical production of hydrogen using earth-abundant materials. Their device is composed of a conductive membrane that has both the role of absorbing the solar radiation and supporting the initial charge separation. Electrons and holes are directed to different sides of the membrane, where two specifically designed organic catalysts assist water reduction and oxidation half-reactions. Their research led to 43 presentations and publications. The team has leveraged their results and successfully bid to become a Department of Energy funded, Energy Innovation Hub called the Joint Center for Artificial Photosynthesis (JCAP). JCAP will receive $122 million over five years to work on generating fuels directly from sunlight.

Professors H.-S. Philip Wong, Peter Peumans, Mark Brongersma, and Yoshio Nishi worked on a new nanowire-based multijunction device. The two key components of the design were a (plasmonic) metallic nanostructured electrode serving as light concentrator and spectral filter, and the absorbing material consisting of an array of vertically aligned nanowire-shaped *p*-*n* junctions with different bandgaps. The metal substrate can split the incident broadband solar spectrum and localize spectral energy in different spatial locations coinciding with the location of nanowires with the optimized bandgap. This challenging concept offers multiple advantages such as the use of low-cost and abundant materials, and parallel connection of the multijunction subcells.

Professors Antonio Marti and Antonio Luque of the Instituto de Energía Solar, Spain, submitted their final report on a program led by Professors Gavin Conibeer and Martin Green of the University of New South Wales. The program is developing a proof-of-concept device of a hot carrier solar cell using abundant and non-toxic nanostructured materials. Due to differences in the starting times of the various sub-contracts under this multi-institutional collaboration, their final report includes all their theoretical studies of the fundamental energy transfer mechanisms between hot electrons and phonons and on the experimental setup requirements for the physical characterization and the measurement of the performance of hot carrier devices.

The only program in Advanced Coal came to a completion this year. Professor Reginald Mitchell led the program on coal energy conversion with aquifer-based sequestration involving Professor Christopher Edwards and Professor Scott Fendorf. The process involves CO_2 capture in inherently stable forms through supercritical oxidation of coal in aquifer-derived water. The products of reaction, including CO_2, are returned in the aqueous solvent to the aquifer.

In the area of advanced materials and catalysts one program was completed this year. Professors Robert Waymouth, Christopher Chidsey, and Daniel Stack developed new classes of molecular electrocatalysts for the efficient oxidation of chemical fuels. A novel click chemistry method to covalently attach catalysts on a variety of functionalized carbonaceous and metal oxide electrodes was developed. This work generated two new families of supported alcohol oxidation electrocatalysts based on ruthenium complexes. As part of their efforts to develop fast oxidation catalysts as potential electrocatalysts, a new family of Pd complexes has been discovered for the oxidation of diols and polyols such as glycerol, a versatile feedstock derived from renewable biomass

Two programs were completed in the area of Advanced Transportation. Professor Josh Thomas of the University of Uppsala, Sweden explored high specific energy lithium ion battery cathodes based on iron silicates, which are both environmentally inert and very inexpensive. Iron silicates have been shown to have high stability but low capacity. This material is being modified to accommodate additional transition metal ions that are capable of transitioning through more than one redox state and therefore incorporate more than one lithium per metal ion, raising capacity. The team successfully demonstrated for the first time the cycling ability of a Li-ion battery "whole-cell" (with a capacity of *ca*. 80 mAh) based on a Li_2FeSiO_4 cathode and a graphite anode. They later also demonstrated the exciting use of Li_2FeSiO_4 as a valuable voltage marker during discharge for $LiFePO_4$. This can prove to be an important product route for Li_2FeSiO_4 into the EV market.

A program led by Professor Yi Cui and Fritz Prinz in Advanced Transportation also reached completion. This program was aimed at developing high-energy-density electrodes for lithium ion batteries for electric vehicles. Close-packed, core-shell nanowire electrode architectures were investigated as a means for using low-cost and high specific energy electrode materials – such as silicon and germanium – that would suffer from poor stability in other configurations. Most of the work was described in the final report last year, but the team was granted a no-cost extension and this year developed a novel inorganic-glue. This inorganic glue method can solve the loss of contact issue in conventional silicon particle anodes and enables successful cycling of various sizes of silicon particles, both nano-particles and micron particles. With a limited capacity of 800 mAh/g, relatively large silicon micron particles can be stably cycled over 200 cycles. The very cheap production of these silicon particle anodes makes the method promising and competitive in the lithium-ion battery industry.