# Introduction to Exploratory Projects – Completed

In addition to deep research into high-risk, high-impact fundamental science and technology, GCEP also funds smaller exploratory efforts. These exploratory projects can be funded for up to one year, and have budget limits of up to $100,000 each. The goal of these projects is to quickly evaluate the feasibility of a novel concept. If such an investigation proves successful, the investigators may apply for regular GCEP funding.

Nine exploratory projects will have reached completion this year in the areas of Hydrogen Production, Distribution and Use, Renewable Energy-Solar, and Renewable Energy-Biomass, $CO_2$ Capture and Separation, $CO_2$ Storage, and Advanced Combustion.

In the area of Renewable Energy-Biomass, Professor Zare's and Maria T. Dulay's work on investigating an immobilized enzyme system for lignocellulosic biomass saccharification reached completion. This project was aimed at enhancing the bioactivity of cellulase enzymes as well as the stability of the enzymes to increase reusability. Enzymes were immobilized in a microenvironment of porous inorganic-organic hybrid sol-gel polymers and this was shown to increase remarkably the bioactivity of the enzymes. The success of this project may eventually lead to an immobilized enzyme system that is highly efficient at hydrolyzing cellulosic polymers and plant cell wall material for biofuels synthesis.

In the area of Hydrogen Production, Distribution and Use, three projects are reaching completion, two of which also fall under the Renewables areas of Biomass and Solar. The project by Professors Swartz's on efficient cell-free hydrogen production from glucose reached the one year completion date. The goal of the project was to develop scaleable technology that will efficiently convert glucose and xylose, the primary products of cellulosic biomass digestion, into hydrogen using a cell-free system. This project has led to the successful engineering of a production organism to achieve increased hydrogenase production at least 10-fold higher than ever before reported. As a consequence of this and further manipulations of the system Professor Swartz and his group have demonstrated hydrogen production rates that suggest commercial hydrogen productivities approximately 10-fold greater than current ethanol productivities on the basis of MJ of fuel value per liter of capacity per unit time.

Professors Mao and Cummings of Stanford University, and Professors Kroon and Peters of TU Delft, have completed a project on high capacity molecular hydrogen storage in novel crystalline solids. This work studied and determined the previously unknown structure of $CH_4(H_2)_4$ using a novel combined theoretical and experimental approach. They have shown that interactions of the hydrogen molecules with the methane sublattice in $CH_4(H_2)_4$ allows the hydrogen molecules to be packed with higher density than solid hydrogen at its normal freezing point, indicating a novel increased interaction in $CH_4(H_2)_4$. This finding provides insight into understanding intermolecular interactions in hydrogen-dense environments has implications for designing high capacity hydrogen storage materials.

Professor Jaramillo's work on nanostructured $MoS_2$ and $WS_2$ for the solar production of hydrogen will also reach completion this year. This work has shown successful synthesis of $MoS_2$ nanoparticles of various sizes using a reverse micelle encapsulation method, and studied their opto-electronic properties for the synthesis of fuels by photoelectrochemistry (PEC). Opto-electronic studies of the supported nanoparticles show significant bandgap enlargement from 1.2 eV to approximately 2 eV. This exploratory work has shown that nanostructured $MoS_2$ is indeed a promising material for the synthesis of fuels from sunlight.

In the area of Renewable Energy-Solar, two projects have reached completion. Professors Gaffney, from the Stanford Linear Accelerator (SLAC) laboratory, and McGehee, from Stanford University, collaborated on a project aimed at solving fundamental disagreements in the scientific community about the effective potential of Multiple-Exciton Generation (MEG) to enhance the photocurrent produced by photovoltaic materials when exposed to photons with energies higher than twice their bandgap. Although their spectroscopic measurements demonstrated MEG in colloidal PbSe quantum dots, the authors concluded that there is still no evidence that MEG could be used to significantly enhance the efficiency of photovoltaic devices.

Professor Paul McIntyre of Stanford University investigated multijunction nanowire solar cells as an alternative to traditional devices using bulk, expensive-to-grow, high-quality semiconductor single crystals. This project was focused on demonstrating Ge nanowire growth using inexpensive metal catalysts which, unlike the standard Au catalyst, do not produce deep carrier traps in the Ge bandgap; the nucleation and growth of dense, vertical Ge nanowire arrays on (111)-oriented polycrystalline Ge thin films on inexpensive glass substrates; and the formation of heterostructure GaAs/Ge nanowires by continuous, locally catalyzed deposition on Ge wires using Ga and As precursors.

In the area of $CO_2$ storage Professors Brown, Bird, Maher, and Mao have completed an exploratory project on geological sequestration of $CO_2$. This work was focused on studying the mechanisms and kinetics of $CO_2$ reactions in mafic and ultramafic rock formations. Key findings from this experimental work and characterization studies of natural analogues are discussed in the report, and have led to submission of an expanded research project proposal using the techniques developed during this exploratory work. The full GCEP proposal is focused on the reactivity of $CO_2$ in both ultramafic/mafic rocks and in saline aquifers.

In the area of Advanced Transportation, Professor Huggins has completed a one year exploratory effort looking at High Voltage Alloys for Lithium Battery Cathodes. The possibility of the use of selected metal and metal-metalloid alloys that have significantly lower weight than the transition metal oxide materials presently used in lithium-ion battery cathodes was experimentally investigated. In this research the new concept of the use of hybrid electrolytes in aqueous electrolytes was developed. It was demonstrated that pairs of electrodes involving the insertion of different, rather than only the same, ions can be used in advanced batteries. This greatly broadens the choice of possible electrode materials, some with appreciably less weight.

In the area of Advanced Combustion, Professor Capelli of Stanford University carried out Fundamental Studies of Plasma Air Separation. This exploratory work investigated the physics necessary to advance the development of a low power, small scale, air separation unit (ASU) based on non-equilibrium plasma discharges (PD-ASU). The preliminarily design and selection of the test geometry of the air passage, plasma electrodes and discharge type; constructing a prototype of the PD-ASU unit; and simulating the unit using commercial software (COMSOL) to improve the separation performance were the main focus of this study.