

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.

Eight exploratory projects were awarded funding last year and are due to finish at the end of August this year.

Professor Matteo Cargnello led a project on low-temperature selective conversion of biomass-derived compounds to fuels and chemicals using electrocatalytic methods. This project was aimed at the conversion of sorbitol, a polyol readily derived from cellulose and hemicellulose, to useful building blocks such as rare sugars and polymer starting materials. The researchers identified the steps required for the electrochemical oxidation of sorbitol in solution on platinum surfaces, thus establishing an area that has seen no or little contribution from past research. These insights will enable production of chemicals from sorbitol with selectivity and rather large productivity. This is an important step towards a promising pathway for the utilization of renewable electricity for the sustainable production of chemicals.

Professors Stacey Bent and Bruce Clemens carried out a project aimed at selective electrochemical ammonia production via electron-limiting catalytic devices. The researchers designed a catalyst-insulator-metal device to improve the efficiency of the nitrogen reduction reaction by interfering with its chief competitor, the hydrogen evolution reaction (HER). This device was able to modulate electron availability through an atomic layer deposited tunneling barrier, which resulted in increased suppression with increased thickness. They also developed an inert condensation synthesis for the catalyst nanoparticles, and demonstrated strategies for improving adhesion at the catalyst-insulator interface.

The goal of Professor Dauskardt's project entitled "Accelerating Scaling to Rapid Open-Air Fabrication of Robust Perovskite Solar Modules" was to accelerate the scaling of high-efficiency perovskite solar modules by employing open-air spray plasma processing and solar reliability. They have been successful in developing rapid spray processing methods for fabricating inorganic charge transport layers, a strategy for removing polymeric organic charge transport layers from the device architecture and facilitating larger area perovskite module fabrication. The combination of these spray plasma processing methods in open-air to form full cells as well as high-voltage integrated perovskite modules stands to greatly reduce process complexity and decrease the energy payback time, enabling the commercialization of perovskite technology.

Professor Fan attempted to harvest energy from the sun and universe, simultaneously and so have the ability to generate heat and provide cooling with the same passive device. In this GCEP project, they report the first experimental demonstration of such simultaneous energy harvesting using a configuration where a solar absorber that is transparent in mid-

infrared is placed above a radiative cooler. The solar absorber is heated to 24°C above ambient temperature and provides a shading mechanism that enables the radiative cooler to reach 29°C below the ambient temperature. This work points to a new avenue for harvesting of renewable energy resources.

Professor Horne's project "LCIG (Leave the Carbon in the Ground) Vitalization of Abandoned Oil Wells for Heat and Electricity Production" proposed a methodology to leave carbon left over from crude oil recovery in the subsurface, and bring the energy to the surface in the form of heat. The thermal energy, heat, can then be used to generate electricity or be utilized directly for space and industry heating. The researchers established numerical models of *in-situ* combustion in oil reservoirs configured with both vertical and horizontal wells. Numerical simulations in different well configurations were conducted and the effects of well pattern, well distance, and air injection rate on the reservoir temperature and gas-water ratio were investigated. In summary, this project showed that leaving the carbon in the ground while vitalizing the abandoned shale wells for heat and electricity production could be achievable.

Professors Majumdar and Chueh, studied entropy stabilized oxides to control the partial oxidation of methane. The goal of this project was to identify materials and a cost-effective process for direct conversion of methane to methanol with high yield and selectivity. They investigated a series of poly-cation oxide materials. These heterogeneous materials have different binding energies on the surface, which allowed control of the kinetics of methane oxidation. This method gave a tunable onset temperature for CO₂ production but led to the formation of only CO₂. Further work focused on photocatalytic conversion, using photons rather than high temperature to activate. Using TiO₂ based materials and H₂O₂ as a model system, the researchers observed the formation of methanol. These results provide the foundation for future work aimed at improving the photocatalytic process and developing new reactor design for improved methanol production for potential commercial application.

Professors Wager and Xu worked on a project entitled "Machine Learning, Renewable Energy, and Electricity Markets". This project was aimed at understanding how to integrate renewables onto the grid considering diverse sources and operators. They considered an alternative approach to experimentation in stochastic systems, where a large number of units interfere with one another. The focus was on the problem of setting supply side payments in a centralized marketplace, where available demand is randomly allocated to a set of available suppliers. The outcome of the research was a method for experimentation that will enable us to design marketplace incentives that encourage individual energy producers to act in a way that is aligned with overall social welfare considerations. As the complexity of renewable energy markets grows, such tools will likely become ever more important in designing energy efficient markets.

Professor Xia and his team worked on the development of microporous polymer membranes for gas separations. They successfully developed a new family of microporous ladder polymers that exhibit >100 higher permeability and comparable or higher selectivity as compared to commercial membranes. These polymers also exhibit

excellent thermal and chemical stability, good mechanical properties, and can be synthesized easily from readily available building blocks. This new synthetic capability to access diverse microporous polymer structures and fundamental understanding of their structure-performance relationships, may allow the development of membranes with tunable gas transport properties and rationally designed polymers for various gas separation applications. This work has led to one publication and a provisional patent application on “Arene-Norbornene-Tröger’s base-Derived Ladder Polymers and Membranes Made Thereof”.