

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.

Four exploratory projects were completed this year.

Professor Jen Wilcox led a project aimed at enhancing hydride thermodynamics through nanostructuring, targets hydrogen storage in nanostructured magnesium based hydrides and investigated the reaction mechanism. Results demonstrated that bulk $\text{Mg}(\text{AlH}_4)_2$ can release hydrogen but its uptake reaction is unfavorable, and bulk $\text{Mg}(\text{AlH}_4)_2$ is metastable with respect to bulk MgH_2 . However, early results indicated that in the cases of nanoparticle systems, hydrogen release and its recharging may be possible by controlling the particle size and temperature, which may facilitate experimental studies to determine the thermodynamically favored reaction pathways for the dehydrogenation and hydrogenation processes of $\text{Mg}(\text{AlH}_4)_2$ nanoparticles. The researchers found that for nanoparticle phases, the reversibility of hydrogen release and recharge may be achieved by changing temperature if the sizes of $\text{Mg}(\text{AlH}_4)_2$ and MgH_2 nanoparticles are less than approximately 2 nm and kept to around 3 ~ 4.5 nm in diameter, respectively under a hydrogen partial pressure of 100 kPa (1 bar). They also demonstrated that by controlling hydrogen partial pressure, larger nanoparticles may have similar reversibility of hydrogen release and recharge compared to that of smaller ones, which might reduce technical problems associated with the synthesis of smaller nanoparticles.

Professor Xiaolin Zheng carried out research aimed at discovering new pathways towards high performance transparent conductive oxides. The researchers studied how a composite microwire array and nanoparticle film structure and application of a rapid high temperature flame doping method (the Sol-flame Method) enhanced the electrical conductivity of solution-processed transparent conductive oxides (TCOs). The goal is to expand the material choice for TCO solar panels at decreased deposition costs. High density and uniform ZnO nanowires and ZnO nanowires coated with ZnO shell films as the base materials for TCO, were prepared and the method to measure the sheet resistance of those films identified. The researchers also found that flame treatment improved the properties of those ZnO nanowires and other metal oxides.

Professors McIntyre and Salleo led an interdisciplinary exploratory project entitled “Enabling Methods and Materials for Stackable Tandem Solar Cells with Polymer Electrolyte Interconnect”. This project studied the use of liquid and solid-state electrolyte interconnects to create Schottky and tandem junction solar cells. This approach avoids the complex fabrication processes required to make tunnel junctions typically required for multijunction photovoltaics. Instead it relies on low temperature, easy to fabricate polymer layers, which can be optimized independently of the semiconductor junctions. During this study three core studies were advanced: the first is

to reproduce and surpass previous performance benchmarks using a liquid electrolyte Schottky junction with crystalline silicon; the second is to use the liquid electrolyte junction in a tandem architecture with amorphous silicon p-i-n junctions, and the third, is to develop and optimize a solid state polymer electrolyte layer to eventually replace the liquid electrolyte in Schottky and multijunction (tandem) architectures. At the conclusion of this one-year project the researchers have successfully created crystalline silicon Schottky solar cells using non-aqueous liquid electrolytes. The best device they have made yielded efficiencies of 9.4% with high open-circuit voltages over 0.6 V, fill factors approaching 70% and photocurrents over 20 mA cm⁻². Device performance for this structure appears to be close to optimal for the given spacer thickness used.

Professor Lindenberg and his research group were awarded funds for an exploratory project entitled, "Optimization of Carrier Transport Processes and Figure of Merit for an Intermediate Band Solar Cell". This exploratory research work was focused on the use of ultrafast terahertz spectroscopy as an all-optical probe of the first steps in carrier transport processes in energy related materials. Intermediate-band materials have the potential to be highly efficient solar cells and can be fabricated by incorporating ultrahigh concentrations of deep-level dopants. A significant focus of this exploratory research was focused on investigating carrier mobilities in polymer-fullerene organic solar cell materials, probing short time hole mobilities in regioregular and regiorandom P3HT:PCBM and the dependence of the mobility on the polymer side chain structure and temperature. Typical transport measurements blur together intermolecular and intramolecular conduction processes, making it difficult to develop an understanding of how disorder on different length scales impacts device performance. These measurements show that intermolecular hopping is only weakly dependent on local disorder within the polymer chain, demonstrating the importance of separating local and intermolecular hopping conduction within organic semiconductor devices. These results challenge and provide new understanding of the microscopic processes that determine the fundamental efficiencies of organic solar cells. This project has led to three peer-reviewed publications.

