

Introduction to Exploratory Projects – Ongoing

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 are currently being funded.

Professor Harold Hwang is focused on solar water splitting and trying to atomically engineer oxide heterostructures for this purpose. In this project, the emphasis is on using atomic scale controlled epitaxial oxide heterostructures as the platform to study and develop fundamental concepts in improving the efficiency of solar water splitting catalysts. The project focuses on: identifying the role of the space charge region in the photocarrier separation process by systematically controlling the thickness and doping density in epitaxial thin films; fabrication of atomic scale surface dipole layers to tune the energy band alignments at the electrolyte/oxide interface; and basic characterization of intrinsic carrier transport properties of visible light harvesting photocatalysts.

Professor Jennifer Wilcox has a project aimed at enhancing hydride thermodynamics through nanostructuring. This project targets hydrogen storage in nanostructured magnesium based hydrides and will investigate the reaction mechanism. The proposed efforts will lead to predictions of the more thermodynamically stable phases as a function of nanoparticle size, temperature and H₂ partial pressure. Understanding the phase stability of the complex hydride nanoparticles requires knowledge of their atomic structure and the thermodynamics of the dehydrogenation/rehydrogenation process. In this proposed exploratory investigation the construction of the phase stability of the nanoparticles of Mg(AlH₄)₂ as a function of size and temperature will be investigated.

Professor Xiaolin Zheng is carrying out research aimed at new pathways towards high performance transparent conductive oxides. The proposed research will study how a composite microwire array and nanoparticle film structure and application of rapid high temperature flame doping method (the Sol-flame Method) can enhance 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. Since the start of the project high density and uniform ZnO nanowires and ZnO nanowires coated with ZnO shell films, as the base materials for TCO have been prepared and the method to measure the sheet resistance of those films identified. As a next step, ZnO microwires will be grown and used as the epitaxial substrates for the ZnO film. Finally, the effect of flame doping on ZnO film on its electrical conductivity will be tested.

Professor Bruce Clemens will spatially engineer delamination layers to create inexpensive and scalable single crystal III-V thin films for photovoltaics and photoelectrochemical water splitting. Environmentally assisted cracking mechanisms within the III-V materials system will be investigated. Single crystal films of GaAs and other III-V materials using MOCVD growth will be grown onto lattice matched growth

substrates, and will be separated from their substrates along the heteroepitaxial interface, producing high-quality, single crystal semiconductor films. This process will be driven at high speeds by applying mechanical stresses to these films in the presence chemical species, which will assist in the crack propagation process. This project will build upon the recent discovery of crack-path control through spatially engineered mechanical properties and chemical exposure, to control the location of the crack to produce smooth, uniform-thickness films. This project will soon be underway.