Introduction to Advanced Materials and Catalysts

The development and advancement of materials is an overarching need in systems that extract, distribute, store or use energy. The performance of these systems depends on the properties of the materials: plastics, coatings, alloys and catalysts are some of the broad classes of materials used in current energy devices. Advancements in these materials optimize energy conversion processes, improve system efficiency, extend lifetime, and reduce CO_2 emissions. Although initially developed for a specific application, material properties may cross-cut to other energy technologies or industries.

GCEP has several projects whose main focus is on materials development. Most of these are officially listed under their application area. Some projects have a materials component to their research. For example, research in the Hydrogen area includes studies of nanomaterials for hydrogen storage. Studies in the CO_2 Separation and Capture area on the development of innovative gas separation membranes involve preparation and testing of materials with highly specific properties. The Solar area is replete with materials research for nanostructured photovoltaic cells. The studies listed above are all materials intensive investigations whose details can be found under their specific application areas in this report.

In addition to these, four projects are underway in the advanced materials and catalysts area. Professors Roger Howe, Jens Norskov and Piero Pianetta are using first-principles simulations to discover materials with ultra-low work functions for energy conversion applications, in particular for high-efficiency thermionic conversions. Since the start of the project in October 2011, progress has been made in three areas: density functional theory (DFT) calculations of the work functions of multi-layer surfaces; fabrication of multilayer surfaces with low work functions; and measurements of surface properties of multi-layer surfaces.

Professor Paul McIntyre and Christopher Chidsey are working on a project entitled, Schottky Tunnel Contacts for Efficient Coupling of Photovoltaics and Catalysts. This interdisciplinary project investigates the performance of nanoscale metal insulator-semiconductor (MIS) contact structures that electrically couple optimized catalysts to high quality semiconductor absorbers in photoelectrochemical (PEC) cells, while chemically protecting the absorbers from oxidation during solar-driven water splitting. This work is making progress and the researchers have designed and are now assembling a small ALD reactor to investigate precursor chemistries for deposition of RuO_2-TiO_2 alloy layers that combine the capabilities of an efficient oxygen evolution reaction (OER) catalyst and a chemical protection layer for an underlying silicon absorber. The goal is to minimize utilization of RuO_2, a rare, but very efficient, OER catalyst.

Professors Daniel Stack and Christopher Chidsey are working towards reduction of carbon dioxide using immobilized dinuclear copper complexes as electrocatalysts. This ongoing research focuses on the development of polynuclear copper catalysts attached to and specifically positioned on inexpensive carbon electrodes for electrocatalytic CO_2 reduction or water oxidation. The proposed research entails ligand synthesis, homogeneous catalyst screening, catalyst imprinting and immobilization, and mechanistic analyses, along with complementary density functional theory (DFT) calculations.

Professors Robert Waymouth and Christopher Chidsey are also working toward the reduction of carbon dioxide. Their approach is through electrohydrogenation to produce a variety of renewable fuels. In the first year of this project, the researchers have tested several well-defined molecular complexes designed to activate and reduce carbon dioxide and alkyl formates. These studies have helped illuminate the electronic and structural features of coordination complexes whose metal and coordinated ligands can function cooperatively to react readily with carbon dioxide or its partial reduction products, such as alkyl formates.