



Thrust 2. Renewable Energy to Products: Sustainable Chemicals for Life

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A shift towards renewable, clean energy, requires that we develop new technologies to harness and utilize this energy across all industries. Arguably, the automotive industry is ahead of the curve with electric vehicles becoming increasingly mainstream. In contrast, the chemical industries lag far behind, still relying on fossil resources and energy to produce products, from fertilizers to fuels to plastics, essential to sustain life for the world's seven billion inhabitants. This thematic thrust seeks to break this paradigm by developing modular, multifunctional catalytic systems that harness renewable energy to generate the products essential for human existence.

Earth abundant sources of the useful C, N, O, and H-containing molecules are small, and typically require high temperatures and/or pressures to activate them to make desired products. For example, ammonia synthesis for fertilizer production feeds the globe but demands 1 % of total global energy, in large part attributable to energy required to activate N₂. The foundational theme of this group's work is to replace such energy intensive thermal and chemical energy driving forces with electrochemical or photochemical energy from renewable resources. This concept additionally enables modular deployment of these technologies for point of use production, alleviating the requirements for large scale distribution and storage of renewable energy.

As another example, while low temperature electrochemical conversion of carbon dioxide to hydrocarbons has been demonstrated, the efficiency of the process plummets dramatically if we try to reach even a small fraction of the productivity required to be commercially viable. To overcome these challenges, this team envisions designing new materials to "collect" reactants to an active site and subsequently react them in potentially multi-step electro-photo-thermal catalytic processes in a "single pot" to selectively produce desired products in high yields. This thrust brings together a cadre of highly active researchers on campus with the requisite complementary expertise to achieve above goals.

Creating an efficient device or product requires a wide diversity of talent that is brought together under this thrust. Accordingly, its faculty members are set to (i) develop novel materials for molecular capture and separation, (ii) envision and synthesize multifunctional catalysts to carry out complex chemical transformations, (iii) conceive and integrate the photoactive and ionically/electronically conductive components to harness renewable energy at reduced temperatures, (iv) engineer and fabricate these modular, intensified devices, (v) analyze the materials and transformations at the molecular and atomic scale with an array of *ex-situ*, *in-situ*, and *operando* techniques, and close the loop through (vi) detailed *ab initio* and data-driven multiscale modeling.