"Fuels from Sunlight" Energy Innovation Hub Selection Announcement
Joint Center for Artificial Photosynthesis (JCAP)
Technical Summary

The Challenge

The design of highly efficient, non-biological, molecular-level energy conversion "machines" that generate fuels directly from sunlight, water, and carbon dioxide is both a formidable challenge and an opportunity that, if realized, could have a revolutionary impact on our energy system. Basic research has already provided enormous advances in our understanding of the subtle and complex photochemistry behind the natural photosynthetic system, and in the use of inorganic photo-catalytic methods to split water or reduce carbon dioxide – key steps in photosynthesis. Yet we still lack sufficient knowledge to design solar fuel generation systems with the required efficiency, scalability, and sustainability to be economically viable.

JCAP Research and Systems Approach

The mission of JCAP is to demonstrate a scalable and cost-effective solar fuels generator that, without use of rare materials or wires, robustly produces fuel from the sun 10 times more efficiently than typical current crops. To achieve this goal, JCAP will address the critical R&D gaps at both the component level and at multiple physical scales from the nanoscale to the operational macroscale, that, when integrated, will comprise a full artificial photosynthetic system prototype.

There is a general consensus that an artificial photosynthetic system must consist of the key elements found in the natural system: materials that efficiently capture and convert sunlight to charge carriers, while providing the voltage to drive fuel-forming electrochemical reactions; catalysts to facilitate both water oxidation and the reduction of carbon dioxide to fuel by photo-generated charge carriers; and a membrane to prevent oxygen from reacting with the energy-rich fuel products.

JCAP researchers will focus on the construction of a solar fuels system based on its requisite components:

- **Light Absorbers**: JCAP will discover and develop light absorbers that consist of robust, photochemically stable, Earth-abundant elements to provide the needed voltage and current density to effect fuel formation from sunlight, water, and carbon dioxide, as the only inputs.
- **Catalysts:** JCAP will discover and develop a variety of catalysts to drive the key fuel-producing reactions of interest, such as oxidation of water and reduction of carbon dioxide to energy-rich fuels.
- **Membranes:** In natural photosynthesis, energy conversion depends upon an interconnected network of membranes that separate the reactants and products, and that provide a physical matrix that supports the whole process. JCAP will design and synthesize photoelectrochemical membrane layers that provide ionic pathways and good optical and light-scattering properties, while remaining impermeable to the product fuels and to oxygen.
- **Linkers:** The design of the artificial system must provide "linkers" that efficiently couple light absorbers and catalysts for optimal control of the rate, yield, and energetics of charge carrier flow at the nanoscale, so that the complete macroscale system can achieve maximum conversion of solar energy into fuel.

JCAP's integrated systems approach to the artificial photosynthesis challenge will consistently drive efforts towards the practical assembly and scale-up of these components to a working prototype:

- **Assembly of Components into a Device:** JCAP will develop the strategies and molecular "tool kits" for linking the various needed individual components into a fully functioning nanoscale artificial photosynthetic assembly.
- **Scale-Up from Nanoscale to Macroscale:** JCAP will develop methods for orienting, assembling, and interconnecting nanoscale functional assemblies into macroscale fully functional materials and systems.
- **Prototype Solar Fuels Generators:** JCAP will develop full macroscale system prototypes that capture all of the critical-length scales and phenomena of importance for device operation, such as fluid flows, feedstock input and output streams, optical input paths, mechanical system properties, and physical form factors.
- **Scalability and Sustainability Analysis:** JCAP will, from inception, analyze all components, materials and chemical inputs, hardware designs, assembly methods, form factors, and system implementations with respect to manufacturability and life-cycle analysis, reuse, and remanufacturing, to ensure that the final operational systems are in fact scalably and sustainably manufacturable.

JCAP Management

JCAP's management structure reflects these research and integration themes: JCAP will have strong central management, with two scientific departments. **The Accelerated Discovery Department** will focus on the means to accelerate the rate of discovery of light absorbers, catalysts, and membranes. **The Science-Based Scale-Up Department** will focus on the scientific underpinnings for linking together the various nano-components into fully functional artificial photosynthetic systems on a length scale of centimeters, and incorporating these photosynthetically active elements into fully operational solar-fuels generators on the 10 cm x 10 cm scale.

JCAP Leadership

DOE's investment in JCAP will establish the world's leading center for the study of artificial photosynthesis. As a true research hub, JCAP will actively incorporate the latest discoveries from the wider scientific community (e.g., from DOE Energy Frontier Research Centers and individual principal investigators) and in turn provide metrics and best-practices benchmarking of catalyst and system performance to the community. JCAP is committed to the rapid transfer of research results to private industry for commercialization.

In addition, JCAP will develop new high-throughput systems, computational tools, and instrumentation to dramatically advance solar fuels R&D: JCAP will develop high-throughput systems for discovering and quantitatively evaluating the performance of new light absorbers, photocatalysts, and catalysts; methods and standards for benchmarking the performance of catalysts, photocatalysts, and full photosynthetic systems; theoretical tools for guiding discovery and scale-up efforts; databases for mining and archiving the results generated by the JCAP Hub; unique and unmatched methods for in situ characterization of catalysts and surfaces at BES-supported light sources; and multiscale modeling of the chemical kinetics, fluid dynamics, and mechanical processes that underlie the systems-level performance of full-scale solar-fuels generators.