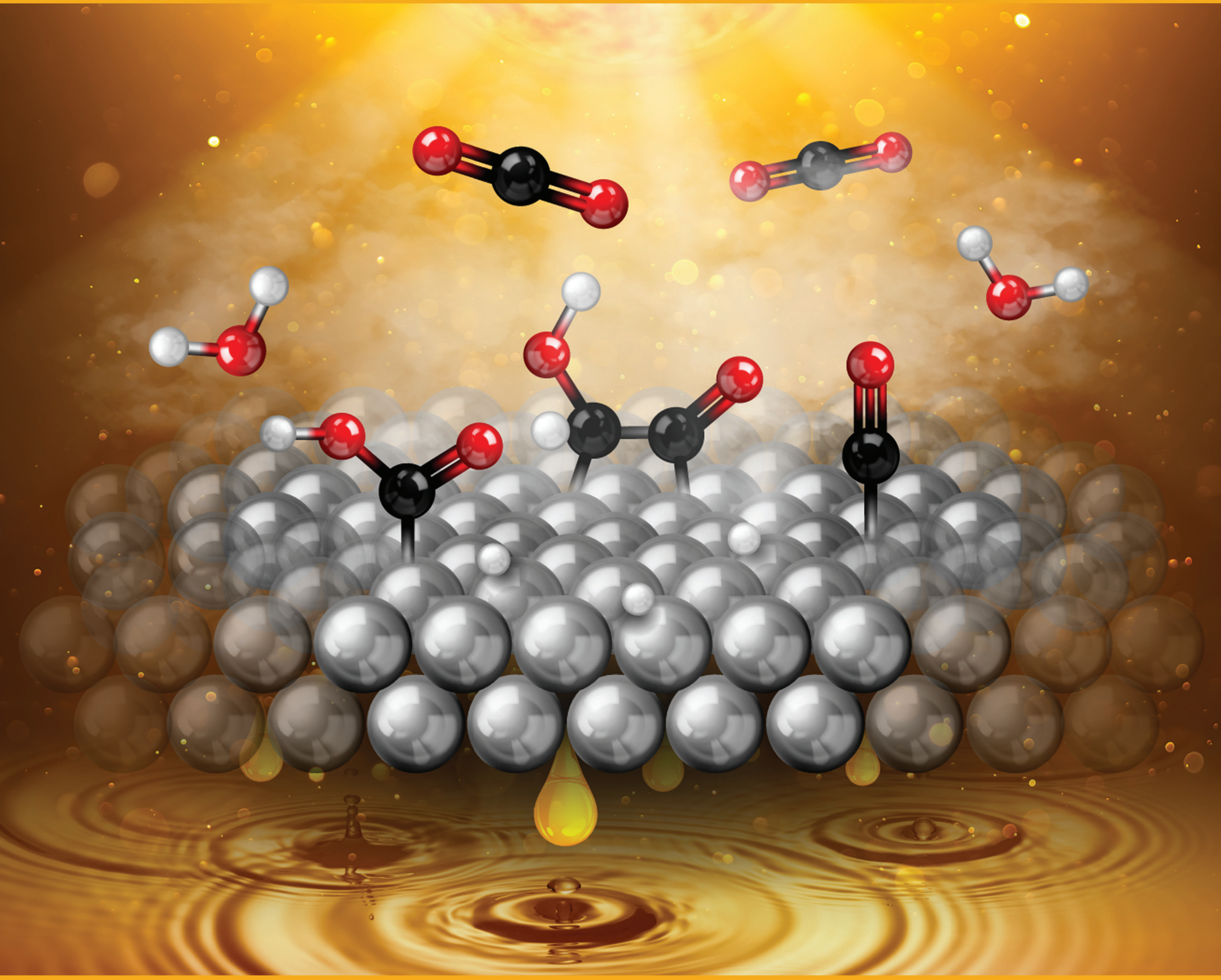
Basic Energy Sciences Roundtable

Liquid Solar Fuels



Report of the Basic Energy Sciences Roundtable on

Liquid Solar Fuels

August 20-21, 2019

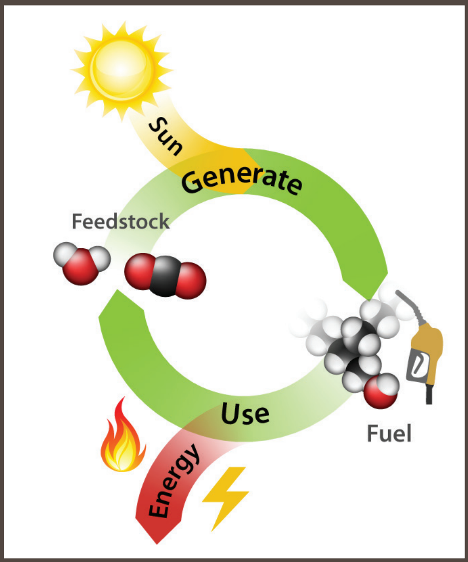
Liquid Solar Fuels—*Fundamental Science to Enable Solar Fuels Beyond Hydrogen*

Sunlight is Earth's most abundant energy resource. Remarkable advances in photovoltaic technologies are allowing society to better capitalize on this resource for electricity generation. Harnessing the power of the sun to produce energy-rich chemicals directly from abundant feedstocks such as water, carbon dioxide (CO_2), and nitrogen (N_2) promises a plentiful supply of sustainable, transportable, and storable solar fuels to meet future US energy needs. Furthermore, solar fuels can provide pathways for efficient chemical energy storage to complement existing electrical energy storage. Solar fuels can also produce diverse chemicals, products, and materials with low environmental impact.

Solar fuels generation—often termed artificial photosynthesis—involves the direct conversion of solar energy to chemical energy using man-made materials and chemical processes. Significant progress has been made to boost the efficiency of solar-driven hydrogen production. Much less progress has been made in the area of liquid solar fuel, an approach that requires chemically transforming CO_2 and other small molecules into promising fuel targets. Hydrocarbons and/or oxygenates produced from CO_2 conversion will be compatible with existing fuels infrastructure. They could also be valuable for production of commodity chemicals and materials. The generation of ammonia and other nitrogen-containing species, which can be used as fuels, fertilizers, and other commodities, presents an opportunity to exploit an extremely abundant feedstock—atmospheric N_2.

The science that underlies solar fuels generation using an artificial photosynthesis approach builds upon decades of sustained fundamental research. Basic research on phenomena in organic and inorganic systems—as well as on the complex biological conversion of sunlight into chemical energy by natural photosynthesis—is advancing the molecular-level understanding of important physical and chemical phenomena such as light absorption, charge generation, electrocatalysis, thermal catalysis, ion and mass transport, and product separations. Light-driven generation of liquid solar fuels requires the coordinated action of a number of phenomena. These processes occur over vastly different time and length scales. Further progress in developing artificial systems for liquid solar fuels production will require new knowledge and advances to control and link individual processes. Components and systems will need to retain their structural and functional properties under operating conditions in real-world environments for significant time periods. Research must identify and advance the scientific principles necessary to achieve selective and efficient fuels production through integration of molecular and material components while ensuring durability.

Basic Energy Sciences held a Roundtable on Liquid Solar Fuels in August 2019 to examine fundamental challenges and research opportunities for generating energy-rich liquids from abundant feedstocks using sunlight as the only energy input. Four Priority Research Opportunities were identified to address critical physical and chemical phenomena required for selective, stable, and efficient direct liquid solar fuels production using an artificial photosynthesis approach. The full report will be available at https://science.osti.gov/bes/Community-Resources/Reports.



Solar fuels offer the opportunity to create transportable and storable energy from feedstocks that are regenerated upon use. As an example, reactions of CO_2 and water driven by sunlight could generate liquid fuels such as oxygenated hydrocarbons. Subsequent use of the fuel to produce electricity or heat energy closes the cycle, regenerating the starting feedstocks of CO_2 and water. With better understanding of the mechanisms of light harvesting and molecular processes (see Priority Research Opportunities), the abundant power of the sun could be combined with a sustainable closed cycle to transform liquid fuel production.

Priority Research Opportunities

- **Understand the mechanisms that underpin constituent durability and performance**

  Key question: *How can molecular-level knowledge of individual processes in solar fuels generation lead to predictive design of components with enhanced lifetime and desired activity?*

  A current impediment to producing solar fuels is the limited lifetime of components. Significant opportunities exist to design, discover, and develop highly performing and durable components, including robust light absorbers with sufficient photovoltages; efficient, stable catalysts with high selectivity; and tailored materials such as membranes and electrolytes to control transport and permeability. A detailed understanding of the thermodynamics, kinetics, and mechanisms of degradation will enable predictive science for durability at the molecular, material, and component levels. New science will also advance strategies to circumvent or counteract processes that reduce component lifetime and performance.

- **Control the catalyst microenvironment to promote selective and efficient fuel production**

  Key question: *How do we probe, understand, and tailor the structure, composition, and dynamics of the local region surrounding catalytic active sites to direct chemical reaction pathways?*

  High selectivity and high activity in the light-driven production of energy-rich fuels present considerable challenges because of the complexity of chemically reducing CO_2 and N_2 as well as oxidizing H_2O. Advances require molecular-level understanding and control of the microenvironment around catalytic sites to direct reactions for key bond-making and bond-breaking steps. Research is needed to probe and control the interactions of catalysts with supports, light absorbers, electrolytes, and other components. It is also critical to understand how the microenvironment can mediate the transport of reactants, products, electrons, protons, and inhibitors to direct reaction pathways determining efficiency, selectivity, and degradation.

- **Bridge the time and length scales of light excitation and chemical transformations**

  Key question: *How can we enable and exploit the direct interaction of solar excitation with chemical change to achieve high selectivity and high efficiency of solar-to-chemical energy conversion?*

  Most approaches to solar fuels generation decouple light absorption and chemical transformations. Significant opportunities exist to capitalize on the direct coupling of light-driven phenomena and chemical processes to enhance overall system performance. Exploiting light–matter interactions could open up new mechanisms to enable selectivity or efficiency that outperform conventional electrochemical reactions or utilize more of the solar spectrum. Fundamental research can realize advantages unique to light-driven fuels generation such as strong electronic coupling or light-induced structural changes.

- **Tailor interactions of complex phenomena to achieve integrated multicomponent systems**

  Key question: *How can the fundamental science of integration advance the predictive design and control of interfaces and processes to enhance the performance, including durability, of solar fuels systems?*

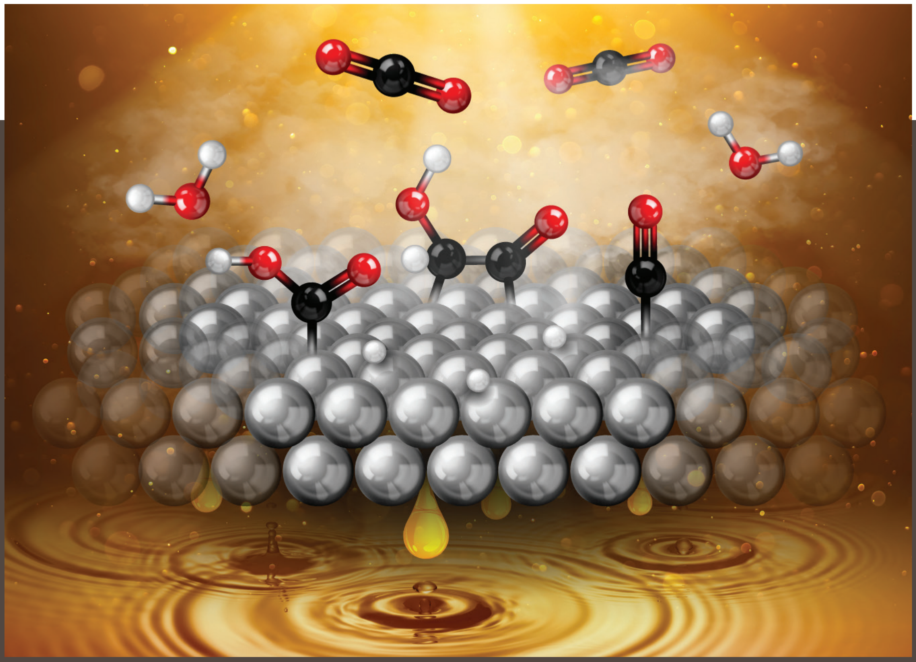
  Integration of individual molecular and material components presents challenges for generating solar fuels because individual elements may not perform the way they do in integrated systems. Fundamental research is needed to provide a mechanistic understanding of how individual multiscale processes interact and affect the function of integrated components. The resulting knowledge of how integration impacts performance, including durability, will guide the development of predictive models and enable the co-design of components for efficient, selective, and durable systems.

Summary

Harnessing the power of the sun to produce liquid solar fuels will provide an abundant supply of sustainable, storable, and transportable energy to meet future US needs. Artificial photosynthesis approaches offer the promise of efficient and scalable generation of liquid fuels using sunlight.

Despite much progress, significant scientific challenges still exist that can be overcome only with fundamental research that facilitates a more complete mechanistic understanding of solar energy capture and conversion as well as integrated component and system performance. The wide range of time and length scales inherent in solar energy capture and conversion present considerable challenges for understanding and controlling light harvesting, energy transfer, charge separation, catalytic reactions, product selectivity, and interfacial processes. Chemical processes and materials properties underlying stability, degradation, and conversion selectivity are central to designing and developing solar fuel system components with desired activity and functionality over extended periods of time and under diverse operating conditions. Moving beyond individual processes and components, the discovery of the scientific principles underpinning integration will enable the design and orchestration of complex systems with desired functionalities. Creating the predictive science for component and systems durability is also essential.

The Priority Research Opportunities identified in this brochure build on foundational studies of solar energy capture and conversion. These opportunities also present new horizons for fundamental chemistry and materials research needed to develop technologies for liquid solar fuels generation. Research will be bolstered by the application of major advances in multiscale theory and modeling, data science, chemical and materials synthesis, and state-of-the-art characterization including ultrafast, high-resolution, and operando capabilities such as those at the US Department of Energy's Office of Science User Facilities.



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DOI: 10.2172/1615599

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