U.S. DEPARTMENT OF ENERGY | Office of Science

Roundtable on Liquid Solar Fuels

Basic Energy Sciences Advisory Committee
July 12, 2019

Bruce Garrett, CSGB Division Director
Basic Energy Sciences
Office of Science, U.S. Department of Energy

BES Roundtable on Liquid Solar Fuels

Workshop Chair: Bill Tumas (NREL)
Co-chairs: Jillian Dempsey (UNC-CH)
Tom Mallouk (U Penn)

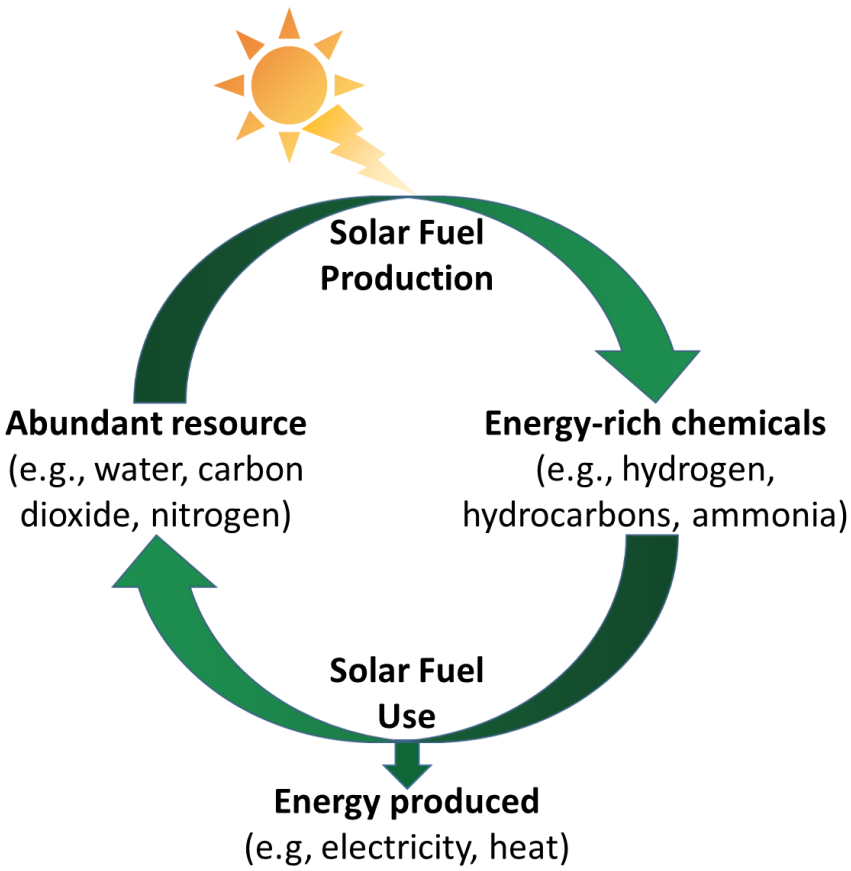
Workshop Date: August 20-21, 2019

Charge:

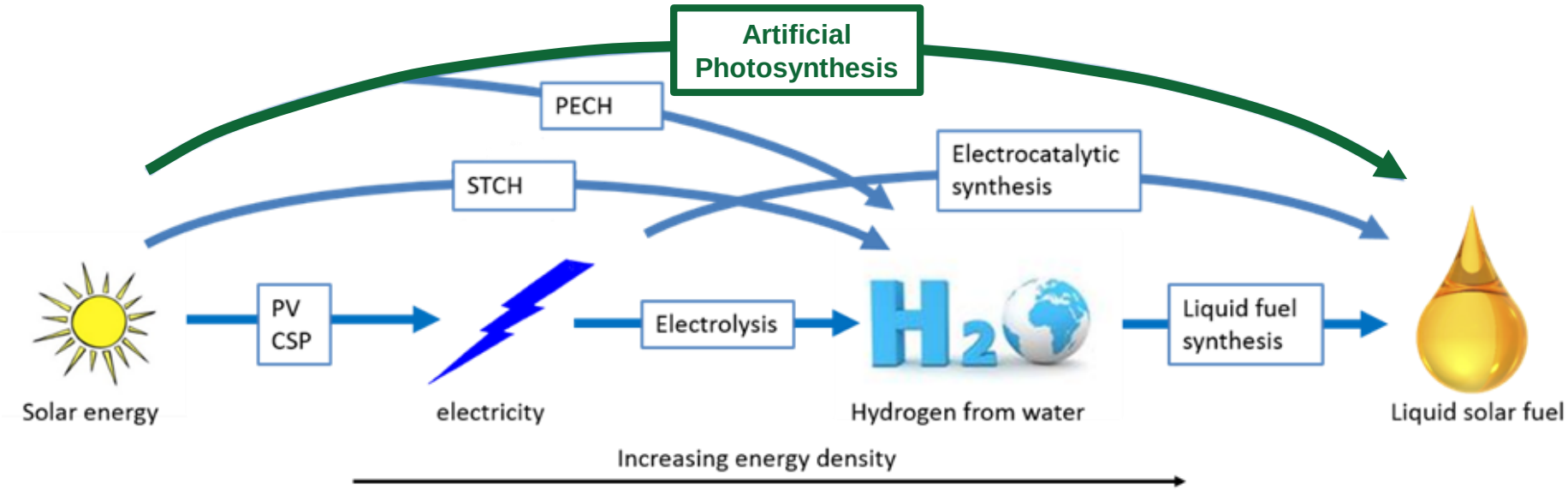
- Assess fundamental research needed to overcome scientific and technical barriers in the generation of *liquid solar fuels*.
- Focus on artificial photosynthesis approaches that can enable direct use of sunlight for liquid fuel production under mild temperature and pressure conditions
- Build on the strong research base in light harvesting, catalysis and interfacial science to identify the most significant fundamental chemical and materials research opportunities in artificial photosynthesis that will provide the scientific foundation for selective, durable, and efficient direct **liquid** solar fuels production

Solar fuels hold the promise of an abundant, sustainable energy supply

- Solar energy is a sustainable and abundant resource capable of meeting future U.S. energy needs
- Solar fuels are energy-rich chemicals generated from abundant feedstocks using sunlight as the only energy input
  - Can operate in a closed cycle
  - Will diversify fuel supply and increase sustainability of energy system
  - Can exploit existing distribution and storage infrastructure

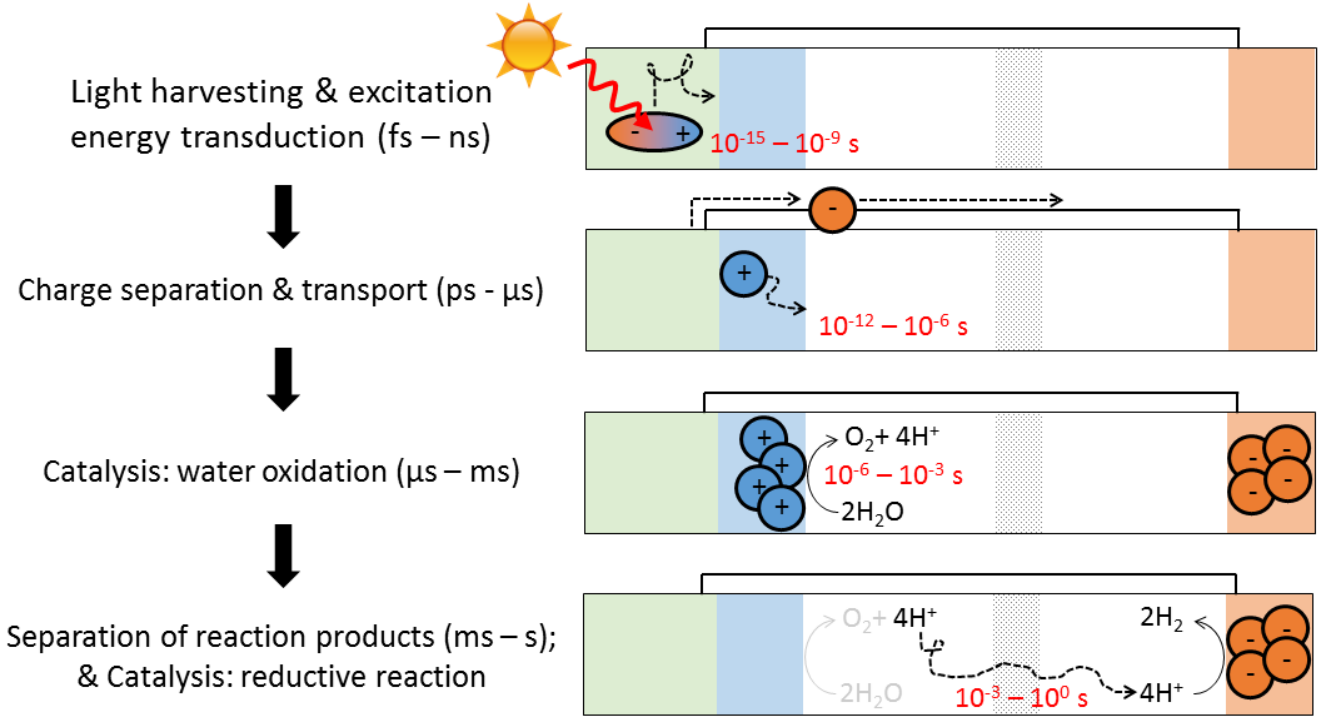


Multiple technological pathways are being considered for converting sunlight to solar fuels



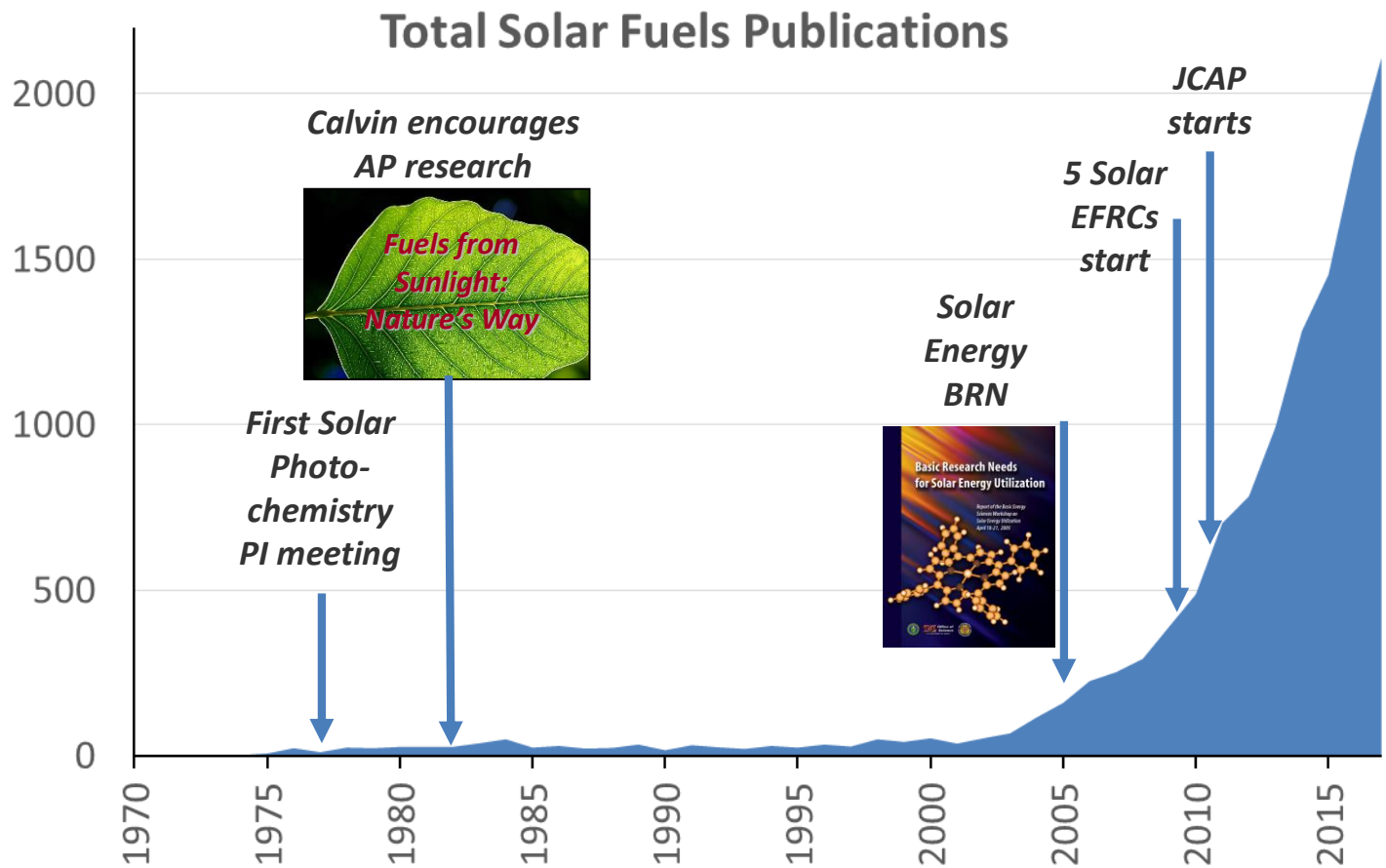
- Indirect routes (e.g., Photovoltaics + Electrolysis) being considered by applied energy offices (e.g., Energy Efficiency & Renewable Energy)
- BES focus is on long-term fundamental research to enable the direct route to liquid solar fuel production – artificial photosynthesis
  - Holds the promise of greater efficiency through integration of multiple processes
  - Provides a pathway to scale technology to the highly-distributed resource

Fundamental processes in artificial photosynthesis present research challenges impeding technology development



- Basic research challenges span length and time scales requiring
  - Understanding, and ultimately control, of individual steps
  - Discovery of functionally active and robust molecules, materials, and components
  - Advancement of nano/meso/macro-scale integration science for assembly of components into complete systems
  - Understanding of (i) competing processes that degrade components and (ii) mechanisms that increase their durability

Solar fuels research is rapidly growing

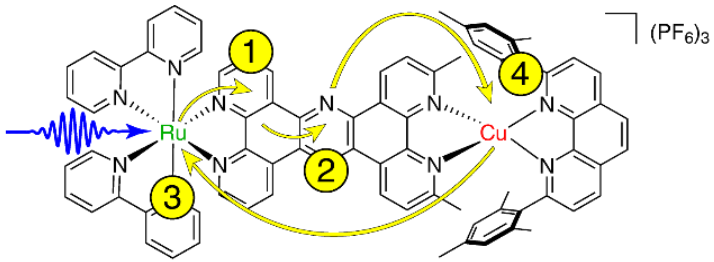


The promise of Solar Fuels has been recognized nationally and internationally – the rapidly increasing research activity indicates its growing importance

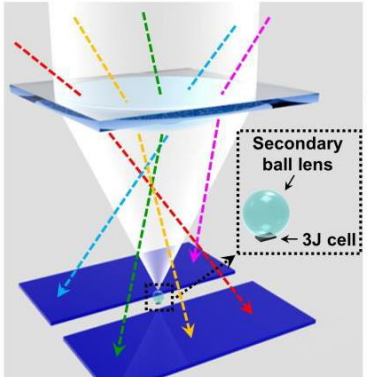
BES support for Solar fuels research spans 4 decades

Multiple funding motifs provide balanced support for BES solar fuels research to address these challenges

- Core programs
  - Provide long-term, stable, renewable support for individual-PI to multi-PI team efforts
  - Focus on advancing difficult fundamental science challenges
- Energy Frontier Research Centers
  - Provide 4-year renewable support for multi-institution, cross-disciplinary efforts
  - Bridge fundamental to use-inspired research to address challenges impeding advances in energy science
- Energy Innovation Hub
  - Provide 5-year renewable support for cross-disciplinary, closely-integrated efforts
  - Identify and overcome scientific barriers and translate knowledge to develop energy systems

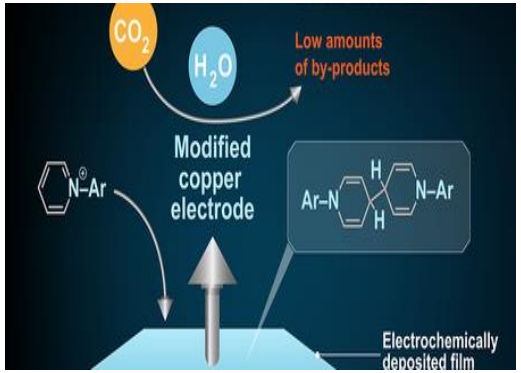


Photoinduced Dynamics



Capturing Both Direct and Diffuse Sunlight For Increased Efficiency

Controlling Selectivity of CO_2 Conversion



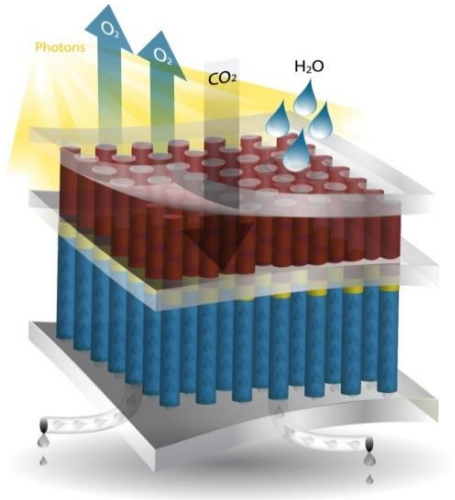
Fuels from Sunlight Energy Innovation Hub

Energy Innovation Hubs

- Multi-investigator, multi-disciplinary integrated centers that focus on overcoming the scientific barriers to development of a complete energy system that has potential for implementation into a transformative energy technology.
- The objective of the Fuels from Sunlight Hub is to develop an effective solar energy to chemical fuel conversion system. The system should operate at an overall efficiency and produce fuel of sufficient energy content to enable transition from bench-top discovery to proof-of-concept prototyping.

Joint Center for Artificial Photosynthesis (JCAP)

- Launched in September 2010 (~$25 M/year for 5 years)
  - Goal**:** Discovery of robust, Earth-abundant light absorbers, catalysts, linkers, membranes, and scale-up science that are required to assemble the components into a complete system that produces fuels from sunlight.
- Renewal in September 2015 ($15 M/year for up to 5 years)
  - Goal**:** Build the scientific foundation for a scalable technology that converts carbon dioxide into renewable transportation fuels, under mild conditions, with only solar added energy.
- Led by Caltech with LBNL as primary partner; additional partners are SLAC, UC San Diego and UC Irvine (Current PI: Harry Atwater)



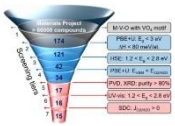
Photoelectrochemical Solar-Fuel Generator

JCAP's First Nine Years…

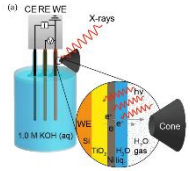
Focus on solar-driven H_2 generation and electrocatalytic CO_2 reduction

Innovative Tools

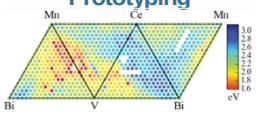
High Throughput Experimentation & Computational Screening



Operando X-ray Science



Benchmarking/ Prototyping



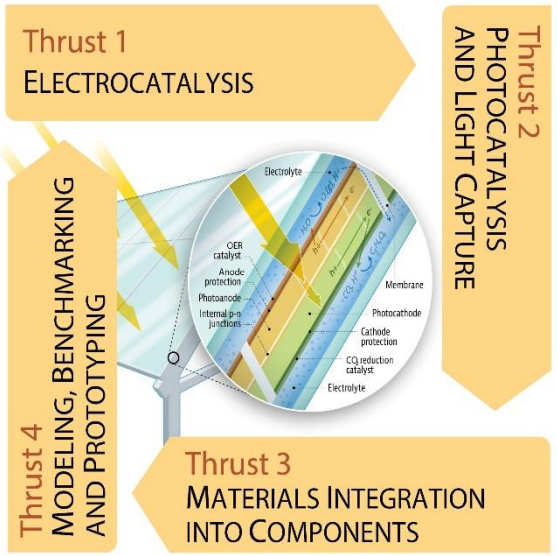
Computational Electrochemistry

Frontier Science Advances

Mechanistic Understanding of Photo-Electro-Catalysis

- Stable visible light absorbers for water splitting
- Conductive protective layers to inhibit photoelectrode corrosion
- High-performance, Ce-rich catalyst for water oxidation
- Influence of catalytic environment on CO_2 reduction products
- Non-Cu electrocatalysts that convert CO_2 to multi-carbon species
- Catalyst features required for efficient integration with photoanodes

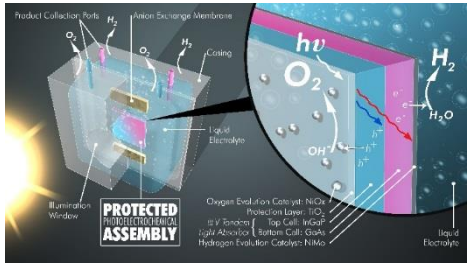
Multi-disciplinary Integrated Approach



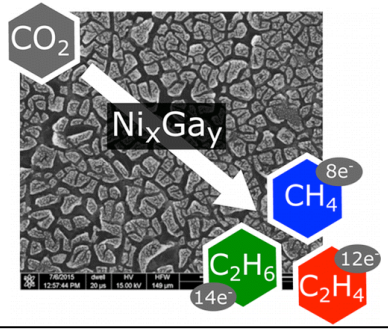
JCAP's Integrated Approach Combines Mechanistic Understanding, Component Discovery, and Systems-level Analysis

Major Technical Achievements

>19% Efficient Solar-Driven H_2 Generation



Selective Electrochemical CO_2 Reduction to Multi-carbon Products



Fundamental Science Outcomes → **Four Research Thrusts** → **Technical Accomplishments**

Future planning for Fuels from Sunlight Hub

- President's request includes $20M for Fuels from Sunlight Hub
  - "… supports fundamental research on solar fuels generation that builds on JCAP's unique capabilities and accomplishments to date"
  - "A competition will be held to solicit new awards of multi-investigator, cross-disciplinary solar fuels research to address emerging new directions as well as long-standing challenges …"
  - "… focus on tackling forefront, fundamental scientific challenges for generating fuels using only sunlight, carbon dioxide, and water as inputs"
  - "Advances in this area will also benefit from consideration of photodriven generation of fuels from molecules other than CO_2"

- House markup includes "not less than $15,000,000 for the Fuels from Sunlight Innovation Hub …"

Need for the Roundtable driven by changing landscape since 2005 Solar Energy BRN; timing driven by upcoming opportunities

Goal: Liquid Solar Fuels Roundtable

- Convene a small group (25) of experts from industry, academia, and national labs to address fundamental challenges to enable artificial photosynthesis for production of liquid solar fuels
- Prepare a factual document to provide the workshop participants with a high-level assessment of the current status of solar fuels
- Identify priority research opportunities (PROs) in which fundamental research over the next 5-10 years could result in a significant impact on advancing artificial photosynthesis
- Prepare a report that captures these possible PROs

Status:

- Chairs, panel leads and participants confirmed
- Date, Location selected: August 20-21, Rockville Hilton (space limited, attendance by invitation only)
- Factual Status document being drafted (delivery by early August) – discuss in webinar before workshop (tentatively mid August)
- Panel topics identified

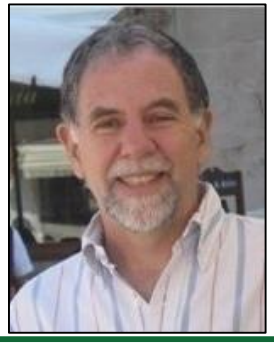
Panel topics focus discussions on fundamental science gaps to achieve efficient, stable, and selective liquid solar fuels

- Science of selectivity and efficiency (Wendy Shaw, PNNL):
  - What are the chemical mechanisms at work in complex electrochemical environments? Using this understanding, can molecular-scale environments – processes, components, and materials – be designed to direct reaction pathways and achieve the needed selectivity and efficiency?
- Science of integration (Kara Bren, U Rochester):
  - How does the dynamic response of a multicomponent system depend on its individual components? Why and how do functions and mechanisms of individual components sometimes change when integrated into a system?
- Science of durability (Shane Ardo, UC Irvine):
  - What mechanisms are involved in the processes that lead to component and multicomponent system degradation as well as those that underlie component reliability and durability, including mechanisms for self-repair and reactivation?
- Crosscutting issues (Andrew Rappe, U Penn):
  - What are the opportunities to accelerate discover and design of innovative processes and materials, such as membranes and catalysts?

Liquid Solar Fuels Roundtable - Format

- Welcome and introductions
- Goals and logistics
- Plenary Presentations
  - *Solar Fuels in Europe* (Leif Hammarstrom, Uppsala U)
  - *Joint Center for Artificial Photosynthesis* (Harry Atwater, Caltech)
- Overview of Liquid Solar Fuels (chairs)
- Breakout panel discussion on each focus area (with cross-cut integrated):
  - Each participant will come prepared to discuss roadblocks, knowledge gaps, research needs, and research opportunities
- Report out on Priority Research Opportunities (PROs)
- Breakout discussions to refine PROs
- Final report out of PROs
- Report writing (afternoon of 2nd day) – writers, panel leads, and chairs stay extra half day to capture input and pull together a rough draft

DOE Basic Energy Sciences (BES) Roundtable on Liquid Solar Fuels



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Panels and Panel Leads:

Science of Selectivity and Efficiency, Wendy Shaw (PNNL): how can we design systems and processes to enable efficient production of targeted liquid fuel molecules in sufficient quantity while limiting unwanted molecules?

Science of Integration, Kara Bren (U Rochester): how do functions and mechanisms of individual components change when integrated into a system?

Science of Durability, Shane Ardo (UC Irvine): what are the mechanisms that lead to degradation and/or reliability/stability of components and multicomponent systems?

Crosscutting Issues, Andrew Rappe (U Penn): what are the new opportunities to discover and design innovative processes and materials?

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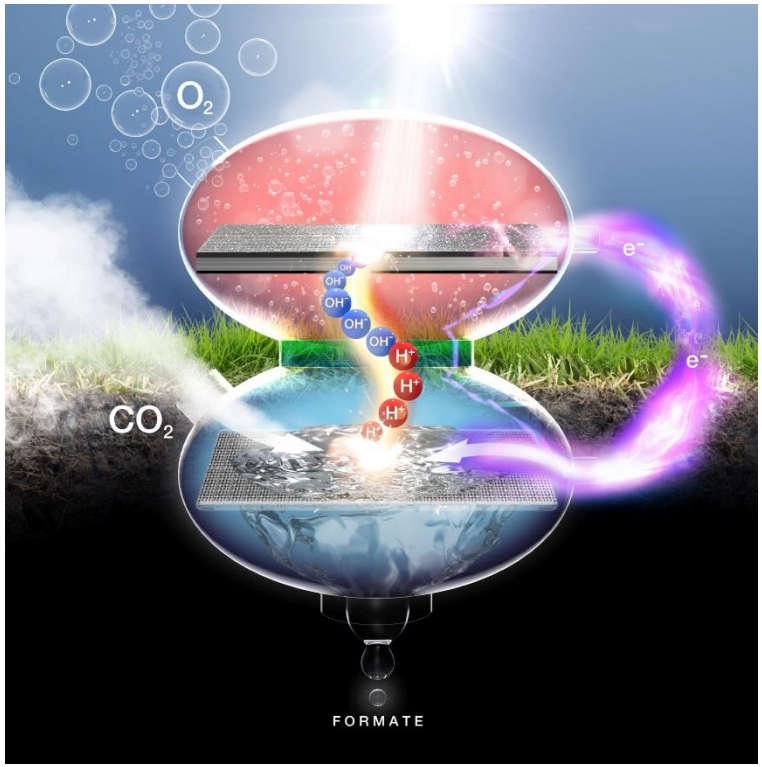
BACKUP

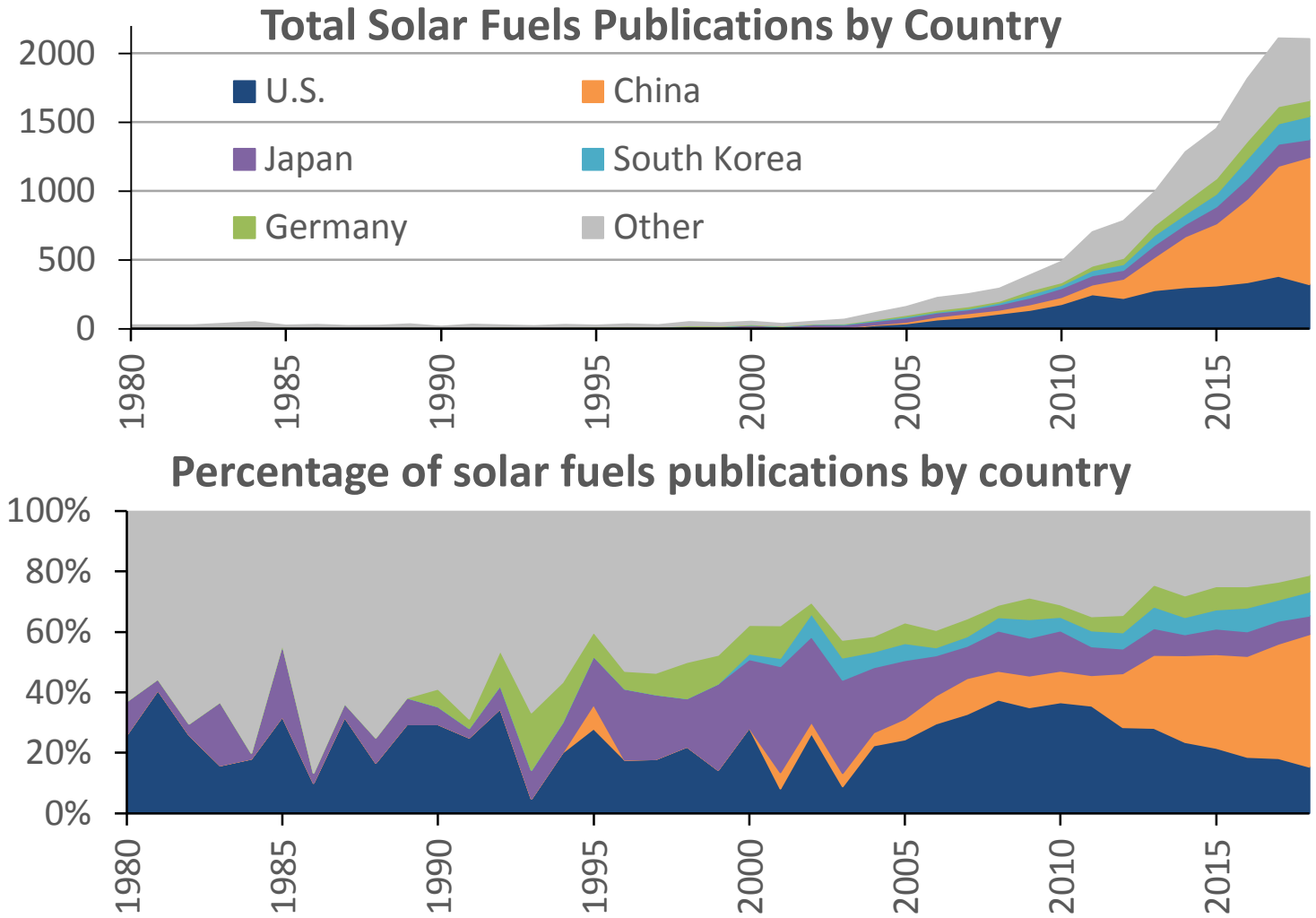
Multiple 'abundant resources' provide promising targets for solar fuels production

- Hydrogen from water splitting
  - Lab prototypes can achieve 19% solar-to-H_2 efficiency with short-term stability
- Hydrocarbons and oxygenates from carbon dioxide reduction
  - Promising recent progress reducing CO_2 to yield specific products, but system integration is a challenge
- Ammonia and hydrazine from nitrogen reduction
  - Longer-term opportunity with large potential impact on reducing energy demands for ammonia production (1-2% of energy use worldwide)



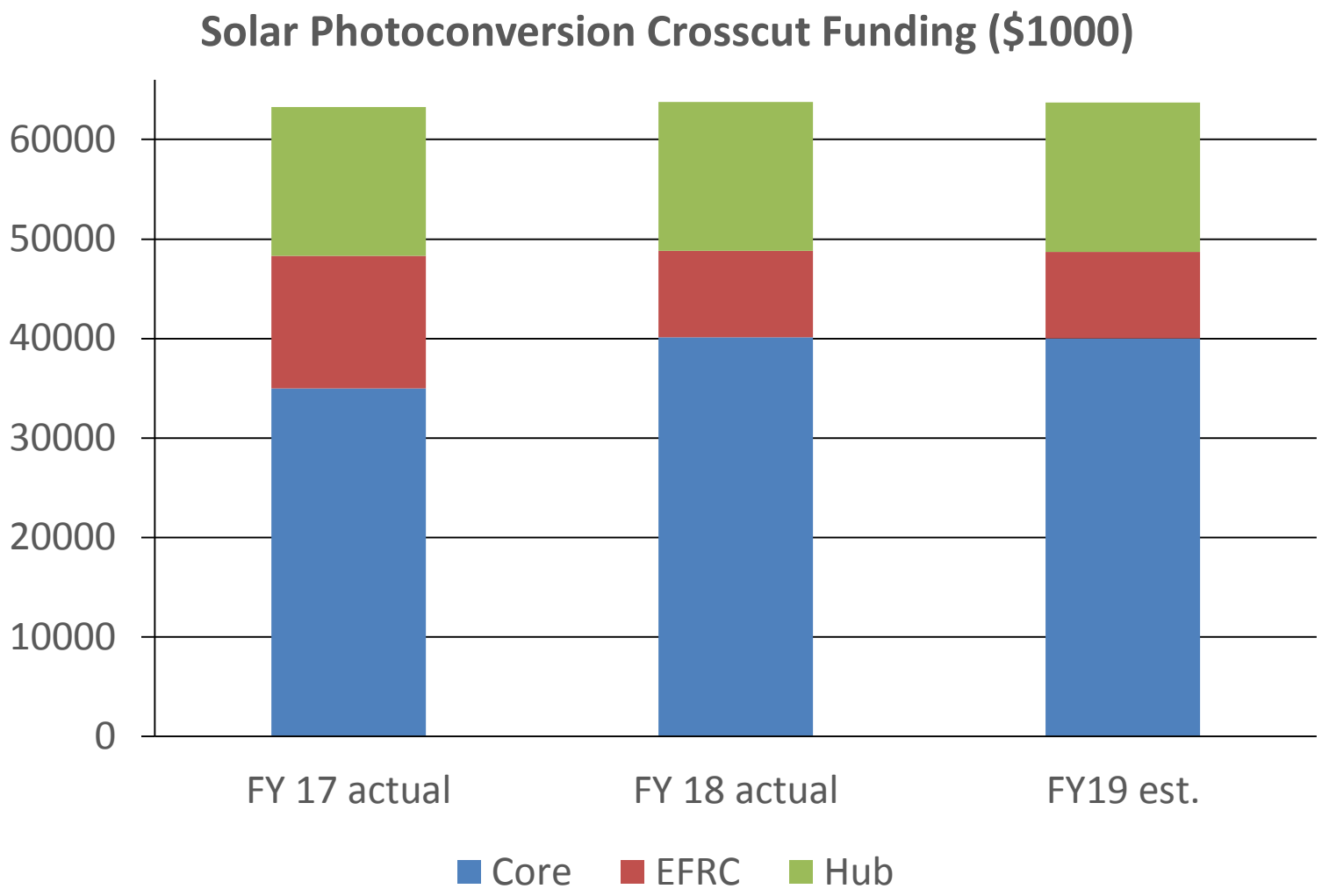
A schematic illustration of the solar-driven CO_2 reduction device

Publications trend indicates a challenge to U.S. leadership in solar fuel



U.S. still leads in impact (e.g., highest cited papers), although falling behind in publications

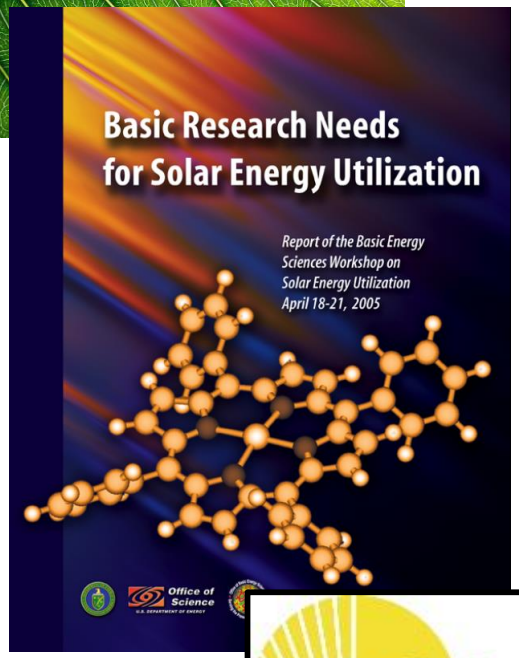
BES continues to invest strategically to advance solar fuels research



Solar fuels research is a long-time focus for BES

- Melvin Calvin (1982)
  - "It is time to build an actual artificial photosynthetic system …"

- BES BRN for Solar Energy Utilization (2005)



- Fuel from Sunlight Energy Innovation Hub – Joint Center for Artificial Photosynthesis (2010)

JCAP
JOINT CENTER FOR
ARTIFICIAL PHOTOSYNTHESIS

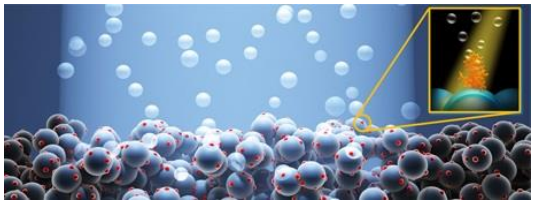
Solar Fuels in Energy Frontier Research Centers

Concept and Implementation

- Multi-investigator, multi-disciplinary centers that tackle fundamental to use-inspired challenges hampering advances in energy science; funding $2-4 M/year for up to 4 years
- The center research topics include areas of chemical and materials sciences that will provide fundamental understanding and tools of potential benefit to solar fuels research.
- In addition, solar fuels has been a central focus of several centers funded in each open competition; currently set of 42 total centers includes 3 center with this direct relevance to solar fuels production.

Current EFRCs Primarily Focused on Solar Fuels

- Alliance for Molecular PhotoElectrode Design for Solar Fuels (U North Carolina)
- Center for Light Energy Activated Redox Processes (Northwestern U)
- Bio-inspired Light-Escalated Chemistry (Princeton U)



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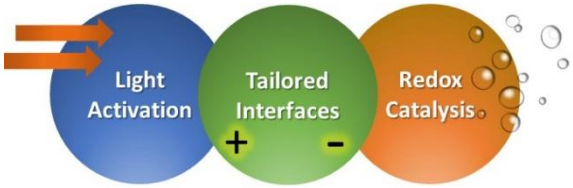

LEAP

BioLEC