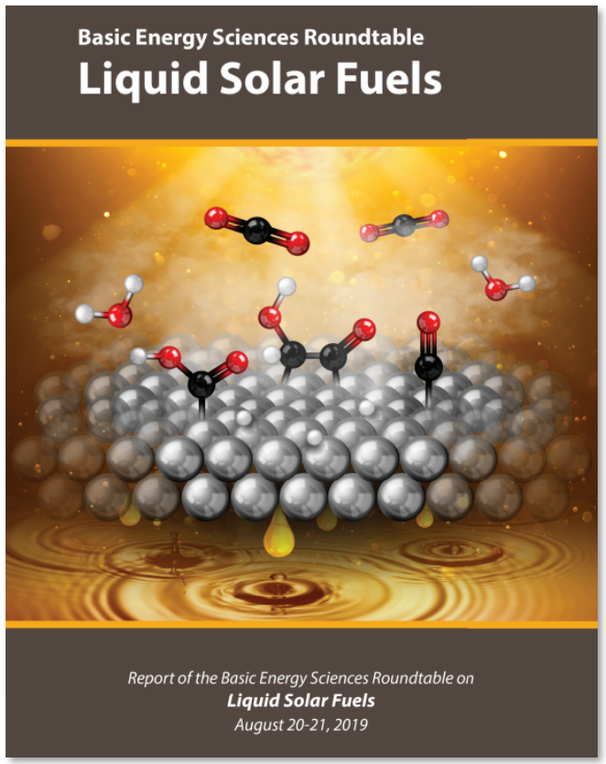
Addressing DOE Priority Research Opportunities

CHASE
Center for Hybrid Approaches in Solar Energy to Liquid Fuels

CHASE HUB WILL ADDRESS EACH DOE PRO IN LIQUID SOLAR FUELS:



U.S. DEPARTMENT OF ENERGY | Office of Science

PRO-1: Understand Mechanisms that Underpin Constituent Durability & Performance

- **CHASE will** develop a fundamental mechanistic understanding of operation and degradation in hybrid photoelectrodes through molecular-level characterization of light-driven catalysis, state-of-the-art ground state and excited state theory, and multi-scale simulations
- **CHASE will** utilize tunability of molecular catalysts, and precise materials synthesis methods, to optimize durability and performance of hybrid photoelectrodes once points of weakness are identified

PRO-2: Control Catalyst Microenvironment to Promote Selective & Efficient Fuel Production

- **CHASE will** tailor catalyst microenvironment on a molecular scale to control local proton activity, electric field, dipole, and lipophilicity to direct reactivity along desired pathways for reduction of CO_2 and N_2 to liquid fuels and for oxidation of water to O_2
- **CHASE will** perform molecular-level characterization through microscopy and spectroscopy to provide insight into mechanisms by which microenvironments optimize catalyst activity, selectivity, durability

PRO-3: Bridge Time and Length Scales of Light Excitation & Chemical Transformations

- **CHASE will** develop strategies to control temporal coupling of multi-proton/multi-electron chemical transformations with light absorption and charge separation processes under solar flux
- **CHASE will** decouple light absorption from catalysis to enable buildup of many charges before rapid multi-proton/multi-electron reactions
- **CHASE will** utilize dual light absorber systems with a semiconductor and a molecular photocatalyst to enable access across high barriers in multi-step pathways to liquid fuels

PRO-4: Tailor Interactions of Complex Phenomena to Achieve Integrated Multicomponent Systems

- **CHASE will** prepare atomically precise hybrid molecule/material photoelectrodes comprised of light-absorbing semiconductor materials and molecular catalysts for liquid solar fuel generation
- **CHASE will** achieve access to high-value liquid fuels, including methanol, ethanol, butanol, high-octane hydrocarbons, ammonia, by spatially-controlled integration of multiple molecular and heterogeneous catalysts working cooperatively in catalytic cascades
- **CHASE will** achieve mechanistic insight into factors that control efficiency, selectivity, durability, in hybrid approaches to liquid solar fuel synthesis