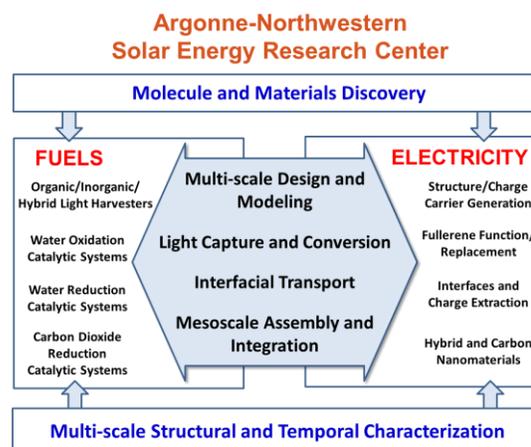


**Argonne-Northwestern Solar Energy Research (ANSER) Center**  
**EFRC Director: Michael R. Wasielewski**  
**Lead Institution: Northwestern University**  
**Start Date: August 2009**

**Mission Statement:** *To revolutionize our understanding of molecules, materials, and methods necessary to create dramatically more efficient technologies for solar fuels and electricity production.*

The ANSER Center is fulfilling this mission by developing a fundamental understanding of solar energy conversion dynamics, by designing and synthesizing new nanoscale architectures with extraordinary functionality, and by linking basic solar energy conversion phenomena across time and space to create emergent energy conversion systems operating with exceptional performance. The ANSER Center addresses a common set of fundamental questions that must be answered to successfully utilize sunlight as a renewable energy source for fuels and electricity. By attacking the common questions intrinsic to solar fuels and electricity in the same research center, the ANSER Center provides opportunities for cross-cutting solutions not possible by addressing only fuels or electricity alone:

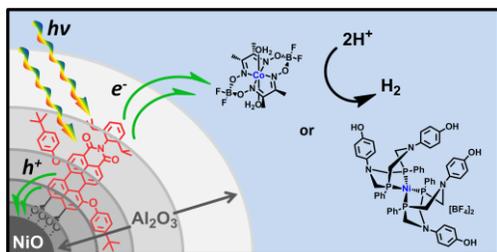
- How can multi-scale predictive theory and computational modeling lead to the design and discovery of novel organic, inorganic, and hybrid systems?
- How do molecular and materials structure and order determine the efficiency of light capture, charge separation, and long-range charge transport?
- What are the fundamental multi-scale temporal and spatial requirements for efficient charge transport across interfaces to deliver multiple redox equivalents to catalysts and electrodes?
- How can molecular and materials properties be tailored to exploit hierarchical assembly for solar fuels and electricity systems scalable from the nanoscale to the mesoscale?



**Fig. 1.** The ANSER Center integrated research program is built on the strengths of molecule and materials discovery and multi-scale structural and temporal characterization.

ANSER Center strengths include molecule and materials discovery and high-resolution spatial and temporal analytical techniques and tools. Specialized X-ray facilities, such as the Advanced Photon Source at Argonne National Laboratory, provide atomic-scale structural information using state-of-the-art *in situ* X-ray absorption and scattering techniques. Ultrafast time-resolved absorption, emission, and vibrational spectroscopy along with time-resolved electron paramagnetic resonance (EPR) spectroscopy and appropriate computational simulation and modeling at ANSER Center laboratories provide detailed information on mechanisms and dynamics.

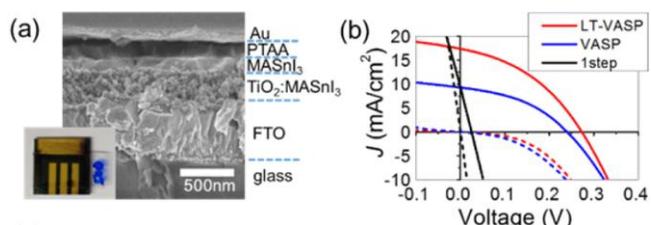
**Subtask 1: Molecules, Materials, and Systems for Solar Fuels.** Our greatest challenge is efficient fuel production at acceptable rates and driving forces. The ANSER Center is employing a hierarchical approach to understanding catalyst and photocatalyst function; thus, requiring a level of integration that cannot be achieved by any single research group. ANSER Center catalyst discovery is strongly hypothesis-driven, nicely complementing but not duplicating the approach of our collaborator, the DOE Joint Center for Artificial Photosynthesis (JCAP) Energy Innovation Hub. The ANSER Center emphasizes catalysts ranging



**Fig. 2.** Photocatalytic proton reduction by molecular catalysts in solution via electron transfer from a purpose-synthesized organic chromophore bound to a semiconductor surface.

from molecules, to clusters, to nanoparticles, to bulk materials that: a) are derived from plentiful elements, b) have promising compositions that are thermodynamically inaccessible as bulk (macroscopic) materials, and c) may enable access to new mechanistic pathways, thereby moving beyond perceived fundamental or practical limits on catalyst performance, including catalyst kinetics and overpotentials. Solar fuels research is exploring and exploiting new ideas about: a) organic/inorganic/hybrid light harvesters, b) water oxidation catalysis, c) water reduction catalysis (e.g. Figure 2), and d) carbon dioxide reduction catalysis.

**Subtask 2: Molecules, Materials, and Systems for Solar Electricity.** Photovoltaic cells fabricated from relatively simple, non-toxic, earth-abundant, mechanically flexible, and low-cost materials offer the prospect of efficient large-scale solar electricity production. Efficiencies have advanced dramatically in the past five years, driven by an ever-increasing, but by no means complete, understanding of the relevant chemistry, materials science, physics, and performance limits. A closely integrated, highly productive interplay of synthesis, characterization at multiple time and length scales, and theoretical analysis and prediction, led to a number of ANSER Center “firsts” in materials design, mechanistic understanding, and performance metrics. Following the same collaborative strategies, ANSER Center solar electricity research continues to explore and exploit new ideas about: a) perovskite-based hybrid solar cells (e.g. Figure 3), b) active layer polymer/small molecule structure-exciton dynamics, c) fullerene acceptor uniqueness and designed replacements, d) new interfacial materials and phenomena, and e) unconventional carbon nanomaterial and metal-organic active layers. ANSER Center research is testing ideas driven by theory to understand at a fundamental level how photovoltaic cell performance is affected by nanoscale/mesoscale architectural-electronic structure relationships in soft-matter and in hybrid soft-matter/hard-matter solar cells, photon capture, exciton creation and decay, exciton dissociation/quenching, and charge transport, electrode microstructure, doping, and surface chemistry. Understanding these phenomena feeds back directly to developing light capture and charge delivery strategies to power solar fuels catalysts as well.



**Fig. 3.** (a) Photo of an encapsulated low-temperature vapor-assisted solution processed device and a cross-sectional scanning electron micrograph of a functional device and (b) current-voltage characteristics of lead-free perovskite devices.

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