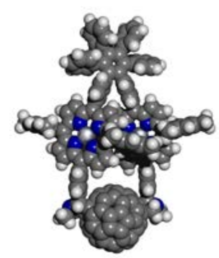
Center for Bio-Inspired Solar Fuel Production (BISfuel)
EFRC Director: Devens Gust
Lead Institution: Arizona State University

Mission Statement*: To construct a complete system for solar-powered production of hydrogen fuel via water splitting. Design principles are drawn from the fundamental concepts that underlie photosynthetic energy conversion.*

Society's heavy reliance on fossil fuels is not sustainable, leads to a variety of geopolitical and economic problems, and contributes to climate change. Sunlight is the most promising renewable source of energy with the capacity to power the world's immense energy economy. The need for a continuous energy supply and energy requirements for transportation necessitate both storage of energy from sunlight in fuel and conversion to electricity. Cost-effective technologies for solar fuel production do not exist, prompting the need for new fundamental science.

Natural photosynthesis harvests solar energy on a scale much larger than that necessary to fulfill human needs. It does so using antenna-reaction center systems that collect sunlight and convert it to electrochemical energy via formation of charge-separated species. This electrochemical potential is coupled to an enzymatic catalyst for water oxidation and to catalysts for reductive chemistry that produce biological fuels such as carbohydrates, lipids, or molecular hydrogen. Photosynthesis is a practical, time-tested natural example of large-scale solar fuel production.

The BISfuel center's approach to the design of a complete system for solar water oxidation and hydrogen production follows the functional blueprint of photosynthesis using designed materials. Collection of sunlight and its conversion to electrochemical potential is performed by artificial antenna-reaction centers. These are constructed using the tools of organic chemistry and components such as porphyrins, fullerenes, and carotenoid polyenes. They incorporate light harvesting, charge separation, photoprotection and regulation. A variety of these have been prepared (an example is shown to the right).


An artificial photo-synthetic reaction center

Working together, BISfuel scientists from a variety of disciplines are pursuing a multi-track approach to creating catalysts. The Center has developed functional water oxidation catalysts using metals such as iridium and cobalt. A more biomimetic approach under investigation is based on a unique, self-assembling, engineered DNA nanostructure that organizes short synthetic peptides in a manner analogous to those in the natural oxygen-evolving complex. These peptides are being used to scaffold a manganese-based catalytic site similar to the natural one using assembly methods found in photosynthesis. In yet another method, peptide-organized water-soluble analogs of the natural photosynthetic oxygen-evolving complex are being developed.

The hydrogen production catalysts under development are synthetic molecules designed using first row transition metals and concepts from natural hydrogenase enzymes. Metal-containing catalytic sites and iron-sulfur sites for storing reduction equivalents are being organized into functional catalysts using synthetic peptides or other supramolecular approaches and interfaced to transparent electrodes.

New transparent, nanostructured, high-surface-area semiconducting porous metal oxide materials are being devised to serve as functional frameworks for organizing the components of the system, separating mutually reactive intermediates, and facilitating electrical communication among components. Several new methods of fabricating such materials have been developed thus far and the ability to incorporate functional molecules has been demonstrated.

DOE National Laboratory resources including SLAC at Stanford, NSLS, and the ALS in Berkeley are being used for X-ray, EXAFS, and electron paramagnetic resonance characterization of the artificial water oxidation and proton reduction catalysts. BISfuel has helped develop the revolutionary new tool of femtosecond X-ray crystallography of nanocrystals for determining the structures of complex and sensitive biological and non-biological molecular materials.

A major challenge is the integration of the various components mentioned above into a unified functional system that is competent to carry out solar-powered water splitting. This requires careful attention both to the thermodynamic and kinetic properties of the catalysts and charge-separation units and to the transport of electrons, protons and other materials among the various subsystems of the complex. Thus, the research has a strong systems engineering component. The Center has demonstrated a functioning system for solar water splitting in the laboratory, but much more research is necessary to evolve a practical process. BISfuel has determined that two photosystems in tandem, à la photosynthesis, will be necessary to achieve useful efficiencies, and such systems are being investigated. Based on the performance of natural photosynthesis, synthetic systems have the potential to produce fuel efficiently from sunlight and water, to be inexpensive, to use earth-abundant elements, and to be a practical solution to humanity's energy problems.

While pursuing this ambitious goal, the Center is uncovering basic scientific knowledge that will point the way to new catalysts for fuel cells, new materials for solar photovoltaics of various kinds, new ways to use DNA and peptides for preparation of artificial enzymes for biomedical and other technological applications, and new fundamental ways of understanding and manipulating matter that will have applications in many different areas of technology. It is also helping to identify ways to modify natural photosynthesis to satisfy better humanity's needs.

Success is possible only through close cooperation among BISfuel scientists from a wide variety of disciplines, including materials science, biochemistry, molecular biology, synthetic organic chemistry, inorganic and bioinorganic chemistry, biology, photochemistry and photophysics. Each BISfuel research subtask focusing on a component of the final system is itself multidisciplinary, and all subtasks work together to assure that the components being developed will ultimately function in the same device. Thus, the Center provides an excellent training opportunity for students and postdoctoral associates who are interested in alternative energy or other multidisciplinary fields.

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Arizona State University	Devens Gust (Director), J.P. Allen, P. Fromme, G. Ghirlanda, A.K. Jones, Y. Liu, A. L. Moore, T. A. Moore, V. Mujica, K. Redding, D.-K. Seo, Ryan Trovitch, H. Yan

Contact: Devens Gust
Regents' Professor
gust@asu.edu
480-965-4547
http://solarfuel.clas.asu.edu/