Center on Nanostructuring for Efficient Energy Conversion (CNEEC)
EFRC Director: Stacey Bent and Fritz Prinz
Lead Institution: Stanford University

Mission Statement: *To understand how nanostructuring can enhance efficiency for energy conversion and to solve fundamental cross-cutting problems in advanced energy conversion and storage systems.*

The overarching goal of the Center is to increase the efficiency of energy conversion by manipulating materials at the nanometer scale. We develop advanced fabrication and characterization methodologies to understand how nanostructuring can optimize light absorption through quantum and optical confinement and improve catalysis through theory-driven design. Each is manipulated to improve performance and efficiency in energy conversion and storage devices.

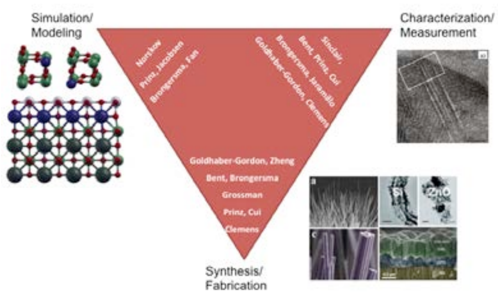

Fig. 1. CNEEC model.

Our research helps provide and expand the scientific foundation of the underlying physical and chemical phenomena shared by a diverse range of energy conversion processes, and exploit them in systems that can lead to break-out high-efficiency, cost-effective energy technologies. Such a multi-disciplinary approach is enabled by the Center structure that provides the intellectual environment and the facilities infrastructure critical to carry out the research projects. A team of CNEEC researchers assembled across disciplines and institutions (see Fig. 1) bring their complementary expertise to bear on these complex but fundamental issues that cut across many energy conversion and storage devices. To pursue its mission, CNEEC has organized its research activities in two interconnected projects:

Project 1. Optical and quantum confinement for light absorption

CNEEC is pioneering the use of optical resonances in high refractive index semiconductor nanostructures for solar applications and in nanometallic (i.e. plasmonic) structures for photoelectrocatalysis. CNEEC is exploring the use of optical resonances in semiconductor and high index oxide nanostructures to ultimately achieve dramatic enhancement in the efficiency of solar absorbers. Properly designed nanostructures and nanostructure-arrays do not require additional light trapping layers as they naturally allow the light to enter and be trapped within the structure. Higher efficiency devices are expected by exploiting these naturally occurring optical (Mie) resonances in semiconductor nanostructures than with the plasmonic approaches pursued thus far. The simple reason for this is that it avoids the undesirable optical (resistive) losses in the nanometallic structures. Despite the tremendous potential, no systematic studies currently exist to optimize ultra thin, nanostructured semiconductor solar absorbers**.** *CNEEC aggressively pursues this new area based on our expertise in the realization of high-efficiency thin film photoelectrochemical (PEC) systems and our leading efforts on the use of the resonances in optical devices.* This project realizes periodic and non-periodic arrangements of nanostructures to enable broadband absorption across the solar spectrum. In collaboration with Project 2, it demonstrates the use of these resonances for the enhancement of oxygen and hydrogen evolution reactions.

In addition to enhancing light absorption by exciting optical resonances in semiconductor nanostructures, CNEEC also exploits quantum size effects to further enhance absorption through bandstructure engineering. This allows one to control where light is absorbed inside the structure using less material. Furthermore, quantum confinement entails a significant modification of the electron and hole wave functions inside a material, leading to the possibility of engineering both the spatial and energetic distribution of charges when designing of next generation solid-state devices. This effort builds upon our recent successes in CNEEC on making and understanding quantum dot structures, including *observing for the first time shape-induced bandgap variations in individual quantum dots*.

Project 2. Atomic scale engineering for catalysis

For all energy conversion technologies that employ catalysts, energy efficiency is directly correlated to catalyst performance. An important goal in CNEEC is to *engineer catalysts with atomic-scale precision* for two key electrochemical energy conversion reactions: (a) water oxidation (oxygen evolution) and (b) hydrogen evolution. Despite decades of research, major technical obstacles still exist in catalyzing these reactions that together effect water-splitting, a potential source of fuel from sunlight, particularly the development of catalysts that are efficient, stable, and that consist of earth-abundant materials. CNEEC takes an approach that triangulates to achieve significant progress: (1) Theory-guided design, where we develop advanced computational models of catalysis on surfaces with predictive power such that one can elucidate specific surface structures, at the level of atoms and electrons, with the desired properties to accelerate the rate of chemical transformations. (2) Inspiration from nature, where we develop methods to study the dynamics of Photosystem II in real time, thereby providing information that can potentially lead to new technologies that rival the capabilities of living things. (3) Atomically-precise methods of catalyst synthesis, where we produce surface structures commensurate with those calculated by theory as well as those that resemble enzymatic catalysts found in nature to be effective for O_2 and H_2 evolution. In this research effort within CNEEC, theory provides guidance as to which surface structures to target, experiments provide feedback to the theory to sharpen and develop the reaction models, and investigation of nature's catalysts help establish design principles for creating new forms of matter with tailored properties for efficient catalysis.

Cross-cutting Themes and Synergy Between Projects

The two projects work together toward the common goal of developing systems that can lead to break-out high-efficiency, cost-effective solar energy-to-fuel technologies. The projects are closely tied together through two mechanisms: (a) physical test systems that integrate light absorption with catalysis, which necessitates the study of interfacial properties and processes that are critical to development of successful absorber-catalyst systems for solar fuel conversion, and (b) the investigation into similar material systems that allow us to leverage the understanding across the projects. CNEEC is working to directly build integrated light absorption structures with catalytic surfaces. The Center pursues studies that cross-cut both projects aimed at understanding interfacial behavior such as defect states, charge transfer properties, and band alignment for the most promising materials discovered in each project. *Our EFRC is aiming to fuse the beneficial effects of quantum and optical confinement in nanostructures to realize higher efficiency photoelectrochemical systems.* In these projects, the length scales that range from the order of 10^2nm (wavelength of light) to 10^1nm (Bohr exciton radius) and 10^0nm (catalytic site dimension) span across both Projects and the physical phenomena they address. The ability to simultaneously build, study, and analyze such integrated nanostructures uniquely offered by CNEEC is crucial for realizing next generation energy systems.

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