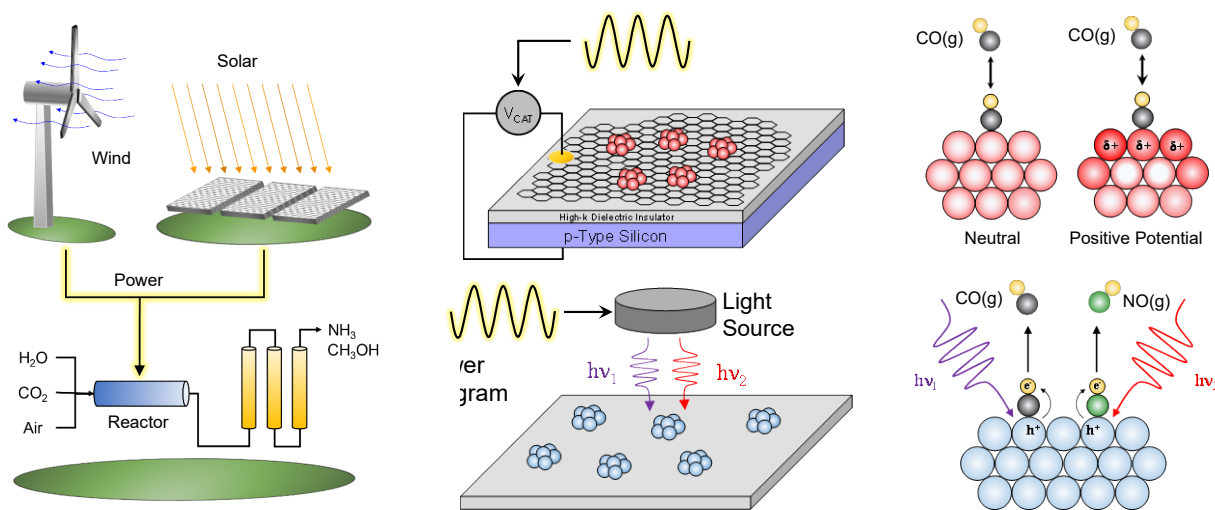


Center for Programmable Energy Catalysis (CPEC)
EFRC Director: Paul J. Dauenhauer
Lead Institution: University of Minnesota
Class: 2022 – 2026

Mission Statement: *To transform how catalysts control energy and accelerate chemistry*

The emergence of low cost distributed power from wind turbines and solar photovoltaics provides attractive possibilities for using renewable electrons to drive thermocatalytic reactions in smaller, more efficient, and geographically-distributed catalytic reactors. To advance this goal, CPEC connects thermocatalysis to electrical power in the novel mechanism of providing power pulses to surface chemistry. The center's central thesis is that dynamic modulation of chemical bonding at catalytic active sites, achieved either by oscillating electron density or by photon-modified adsorbate-catalyst bonds, accelerates surface chemistry and provides control over reaction pathways to targeted products. Exciting results emerging in just the past few years have established the programmable concept and its promise for controlling surface chemistry. However, much remains to be discovered concerning programmable catalysis, its mechanisms, and fundamental behaviors. *The uniqueness of CPEC is its focus on fundamentals of complex forced dynamic surface kinetics* to understand the interplay between molecular-scale interactions, active site design, light and charge perturbations, and the dynamic changes in surface structure and adsorbate composition.



The center addresses the following integrative research objectives that advance fundamental understanding of programmable catalysis (i.e., catalysts perturbed with time).

- Understand charge distribution in catalyst active surfaces and sites under forced perturbation with light or charge.
- Construct reaction models that predict dynamic electronic perturbation of catalysts
- Understand programmable catalyst design and fabrication principles for high surface area and large active site density while retaining catalyst perturbation and dynamic enhancement
- Develop optimization strategies for predicting adsorbate/site/perturbation combinations *and* optimal oscillatory catalyst perturbations to accelerate and control energy-relevant chemistries

CPEC brings together expertise in heterogeneous catalysis, computational chemistry, and materials synthesis to create new catalytic devices that respond to light and charge. These two approaches to applying power locally to the surface have the commonality of oscillatory energy pathways of reacting molecules. Principles developed for one type of energy delivery mechanism apply to others. While the research addresses specific problems, general understanding of this new field of programmable catalyst will be developed in parallel to expand basic principles to a broader field of dynamic catalysts.

The center will establish new methods of operating catalysts dynamically via applied pulses of light with varying intensity, wavelength, and temporal application. Design of catalyst surfaces will be integrated with a focus on understanding the absorption of light and its effect on surface molecules and their reactions. This approach will identify new oscillatory conditions that efficiently use light to direct reaction pathways and accelerate reactions.

The center will also pursue fundamental understanding of a new thermocatalytic device called a 'catalytic condenser.' Comprised of an electrical insulator separating two conductive films, one of which is the catalyst layer, the condenser stabilizes charge (electrons or holes) at the catalyst surface, thereby altering the catalytic reaction. Research skills in materials synthesis and device design, computational chemistry, experimental kinetics, and reaction simulation will pursue an integrated approach to understanding the mechanisms of using charge to control chemistry, leading to faster and more controllable reactions beyond existing catalytic limits.

Center for Programmable Energy Catalysis (CPEC)	
University of Minnesota	Paul Dauenhauer (Director), Aditya Bhan, Matthew Neurock, C. Daniel Frisbie, Bharat Jalan
University of California Santa Barbara	Susannah Scott (Deputy Director), Phil Christopher Michael Gordon
University of Michigan	Eranda Nikolla
Clemson University	Rachel Getman
Massachusetts Institute of Technology	Yuriy Roman
University of Massachusetts Amherst	Omar Abdelrahman
University of Houston	Lars Grabow

Contact: Paul Dauenhauer, Director & Professor, cpec@umn.edu
612-624-0159, www.cpec.umn.edu

Instructions

Provide a two-page technical description of the EFRC's research written for a scientifically literate audience. The use of figures is encouraged. Replace **blue text** with the appropriate information and change the font color back to **black**. Page formatting must include 1-inch margins on each side and the use of 11 pt Calibri. Do not change the blank line between the header, mission statement, body, staffing table, or contact information. Space between paragraphs in the body and other use of white space/formatting that enhances the readability is strongly encouraged. Please send your technical summary with the naming convention [EFRC acronym_technical_summary_year-month] as a word document (*.docx) to Shawn Chen (shawn.chen@science.doe.gov). The individual word documents will be combined into a single technical summary document for the EFRC program. Therefore, the two-page limit and formatting requirements will be strictly enforced. If you want to ensure the technical summary renders correctly, you may submit a PDF version in addition to the word document.