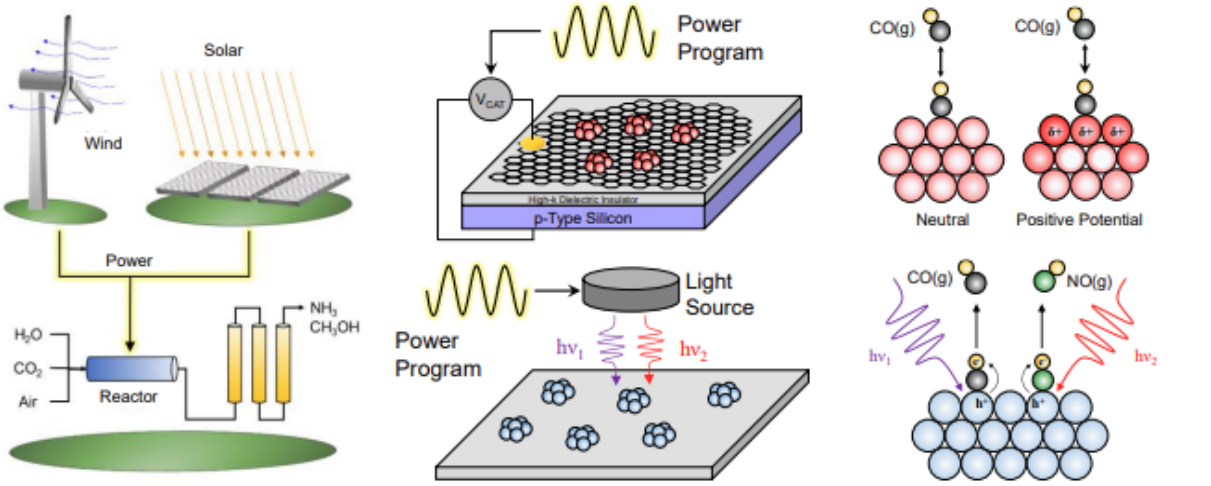
Center for Programmable Energy Catalysis (CPEC)
EFRC Director: Paul Dauenhauer
Lead Institution: University of Minnesota
Class: 2022 – 2026

Mission Statement*: To transform how catalysts control energy, and to 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.

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