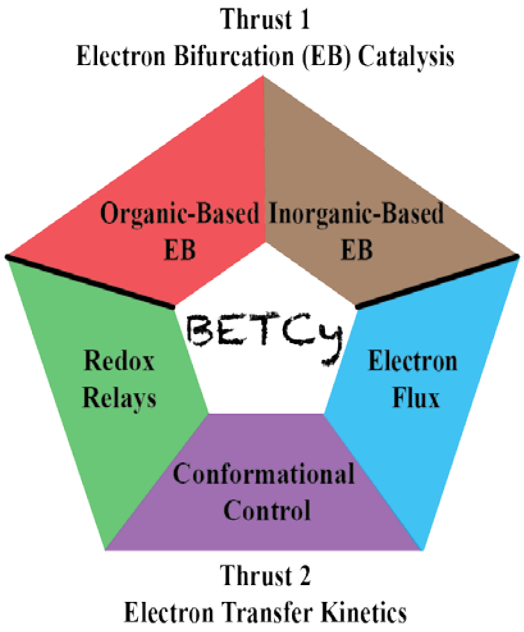
Biological Electron Transfer and Catalysis Center (BETCy)
EFRC Director: John Peters
Lead Institution: Washington State University
Class: 2014 – 2020

Mission Statement*: To understand the means by which biology controls the kinetics and thermodynamics of electron bifurcation at both organic and inorganic centers through electron transfer relays, allosteric coupling, and cooperative conformational dynamics.*

The focus of the Biological Electron Transfer and Catalysis (*BETCy*) EFRC research is elucidating mechanisms of conversion of electrochemical potential into chemical bond energy and is organized into two integrated Thrusts: Electron Bifurcation Catalysis and Electron Transfer Kinetics.



We are developing a collective knowledge of metalloenzymes as models for redox reactions by applying physical science and computational tools to characterize biochemical reactions catalyzed by multi-subunit enzymes harboring arrays of iron-sulfur clusters and flavin cofactors. Understanding these mechanisms is central to overcoming the thermodynamic barriers that currently limit production of reduced products and fuels.

Biological systems have elegant strategies for converting electrochemical potential energy into chemical bond energy (e.g., C-H, H-H, and N-H) stored in reduced compounds that can serve as advanced biofuels. One significant limitation for the production of highly reduced compounds is that their production in natural and industrial processes relies on low oxidation-reduction potential chemicals as feedstocks. However, unique biochemical strategies exist to generate pools of reducing equivalents that can serve as a source of electrons for chemical bond formation from low oxidation-reduction potential feedstocks.

We are focusing on a newly discovered biochemical mechanism termed “electron bifurcation”, which upgrades electrochemical potential by effectively coupling endergonic and exergonic reactions in an overall thermodynamically favorable process. The underlying mechanistic details governing electron bifurcation are, however, still poorly understood and a more in-depth understanding of this phenomenon could lead to “game changing” and transformational advances in strategies to direct electron flow. These studies provide a blueprint for bio-inspired, multi-electron catalytic processes that can ultimately utilize electrons of varying reduction potentials to drive chemical reactions. We are also working to elucidate how biology uses a combination of chemical bond energy and electrochemical potential to accomplish very difficult, low potential reduction reactions (e.g., CO_2 and N_2 reduction) using electron donors of modest reduction potentials.

The goal of the *BETCy* EFRC is to provide a fundamental understanding of mechanisms to overcome key thermodynamic barriers that limit the production of reduced products where energy is stored in the form of C-H, H-H, and N-H bonds. The two interrelated research Thrusts of the *BETCy* EFRC emphasize mechanisms of electron bifurcation in driving low potential oxidation-reduction reactions. The research

of the *BETCy* EFRC builds on recent seminal discoveries in biology and provides the basis for attacking key knowledge gaps and expanding the knowledge base that is essential for realizing the true potential of bioenergy and bio-inspired catalysis as prominent components of the global energy production portfolio. We have assembled a strong team of investigators with complementary research interests and technical skills to accomplish the proposed interdisciplinary tasks. The work is having a profound scientific impact on understanding and predicting matter and energy at the atomic level and in generating a blueprint for efficient control of electron flow into energy products and chemicals.

The work is directly in line with and addresses three of the five Basic Energy Sciences Advisory Committee (BESAC) Grand Challenges including: *1. Control of material processes at the level of electrons, 2. Design and perfect atom and energy efficient synthesis of revolutionary new forms of matter with tailored properties, 3. Characterize and control matter away, far away, from equilibrium* (which is the essence of electron bifurcation reactions). In addition, the proposed *BETCy* EFRC goals embrace the Basic Research Needs (BRNs) outlined in the BES Workshop Report on *Catalysis for Energy*, and makes strong connections with the *Hydrogen Economy* and *Solar Energy Utilization* BRNs. The BETCy EFRC will address its scientific aims using advanced tools and technical approaches in support of the DOE-BES Transformative Opportunities: (1) Mastering Hierarchical Architectures and Beyond Equilibrium Matter, (2) Beyond Ideal Materials and Systems: Understanding the Critical Roles of Heterogeneity, Interfaces, and Disorder, (3) Revolutionary Advances in Models, Mathematics, Algorithms, Data, and Computing, and (4) Exploiting Transformative Advances in Imaging Capabilities across Multiple Scales. Oxidoreductase enzymes couple electrochemical potential to drive chemical transformations using complex architectures that integrate electron/proton circuits to enable the flow of matter over wide-ranging spatial and temporal scales. The complexity of scale presents an enormous technical barrier to elucidating functional principles of enzymes and exploiting their designs to realize transformative reactions. To address this critical issue, the BETCy EFRC team has developed experimental and theoretical methods at the forefront of redox reaction dynamics that enable measurements and interpretation of electron flow through enzyme circuits on the timescales of individual reaction steps.

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