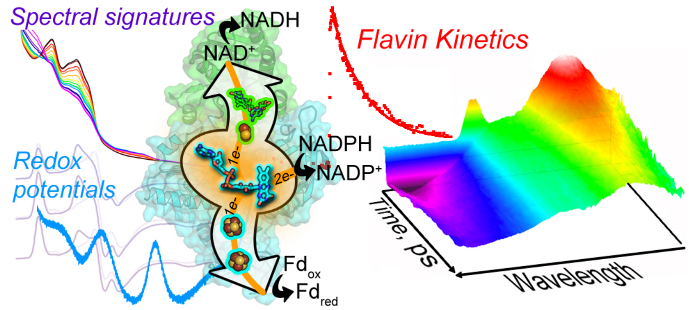
BETCy EFRC scientists discover mechanistic details of electron bifurcation.

In a new publication, BETCy scientists have uncovered some of the hidden mechanistic details of electron bifurcation. Bifurcating enzymes are able to take energy from one source and split it into two pathways in order to produce two different high-energy compounds, one of which is difficult to make. This process allows certain enzymes to harness energy from chemical reactions that previously would have been sloughed off as unusable heat. Understanding this process - which maximizes the efficiency of reactions at the molecular level - could affect everything from synthetic biology to fuel and chemical production.



The publication, "[Mechanistic insights into energy conservation by flavin-based electron bifurcation]" was published online 10 April 2017 in the journal *Nature Chemical Biology*.

By leveraging a multitude of biophysical techniques in five of BETCy's laboratories, researchers were able to deduce the energy landscape by which bifurcation occurs in the transhydrogenase enzyme, Nfn. An extremely short-lived flavin intermediate (10 picoseconds) was observed for the first time and was key to unraveling the mechanism of bifurcation at unique flavin sites. This short lifetime is a requirement that ensures electrons are transferred to the endergonic branch within Nfn so that the high-energy chemical reaction occurs. The integrated nature of BETCy helped drive these technical advances, highlighting the more than one volt of electrochemical potential that Nfn generates during the catalytic mechanism. This unprecedented range of thermodynamic driving force accounts for the unique chemical reactions that are catalyzed by bifurcating enzymes.

"These enzymes are actually quite savvy," said lead-author Cara Lubner of NREL. "Because they couple the reactions in such a way as to conserve energy, it is a very efficient process with little waste."

Lubner

Adams

Mike Adams of the University of Georgia, co-author of the paper, said that typically the fuels we use for transportation or industry originate from the burning of high-energy chemicals—those that are rich in electrons, like coal, natural gas, ethanol and gasoline. Likewise, when the human body metabolizes food, which is also electron-rich, we receive cellular energy to stay alive, and the heat that is given off in the process maintains our body temperature.

“However, in terms of chemistry, releasing energy from high-energy electrons as heat is a wasteful process,” said Adams. “It would be much more beneficial if you could store those high-energy electrons in another chemical, particularly if you are trying to make a fuel.”

“This really opens up the field of energy-related biochemistry,” said John Peters, BETCy EFRC director. “This work has groundbreaking implications. It could allow you to use materials you couldn’t normally use for energy. We could find ways to use both high-quality and low-quality feedstocks to get fuel.”

Peters