Understanding Charge Separation and Transfer at Interfaces in Energy Materials (EFRC:CST)
EFRC Director: Peter J. Rossky
Lead Institution: University of Texas at Austin

Mission Statement*: To pursue fundamental research on charge transfer processes that underpin the function of highly promising molecular materials for photovoltaic and electrical energy storage applications.*

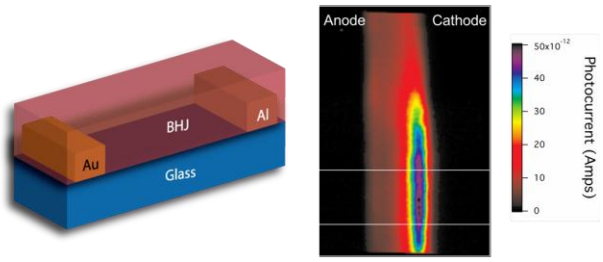
Solar energy conversion and storage are two critical components of a forward-looking strategy to achieve U.S. energy security. This EFRC focuses on a fundamental scientific challenge associated with the development of both organic photovoltaic (OPV) and electrical energy storage (EES) technologies: To understand interfacial charge separation and transfer processes in nanostructured materials at a mechanistic and atomistic level. Progress to date in this area has been limited, in part, by the structural complexity of these materials. They are heterogeneous on the nanoscale, so that conventional probe technique measurements on the meso and bulk scales are incapable of revealing the nano-structural character of these material interfaces, intrinsically limiting the establishment of the structure-property relationships governing these materials for OPV and EES applications. In addition, reliable and feasible theoretical and computational modeling methodologies for describing interfacial charge separation and transfer dynamics in nanostructured materials have not been available. The unique size scale demands that one bridge theoretical approaches between the electronic structure of localized molecular systems and the morphological structure of disordered condensed phase systems. The EFRC:CST was established specifically to overcome these difficulties and hence to markedly advance the fundamental understanding of these charge separation and transfer processes. Three highly coordinated and focused scientific approaches have been implemented:

- Approach 1: The EFRC:CST supports a set of coordinated research projects focused on the design and synthesis of model interfacial prototypes that climb the ladder of complexity from single molecules and single crystals to bulk heterojunctions. These model systems serve as the basis for a divide-and-conquer strategy in experimentally and theoretically unraveling the complex charge separation and transfer mechanisms in nanostructured materials.
- Approach 2: The EFRC:CST is developing state-of-the-art imaging and spectroscopic tools, ranging from single particle spectroscopy/microscopy to in-situ nonlinear optical spectroscopy, to make correlated measurements of structure and charge separation/transfer processes on the multiple size scales present in the model systems developed in Approach 1.
- Approach 3: The EFRC:CST is advancing theoretical and computational methods in the comprehensive calculation and modeling of interfacial charge separation and transfer mechanisms. Via careful coordination with Approaches 1 & 2, these theoretical/computational efforts are providing insights into the structure of nanomaterial systems, the electronic properties of model interfaces, nonadiabatic charge transfer dynamics, and rate processes at multiple material length and time scales.

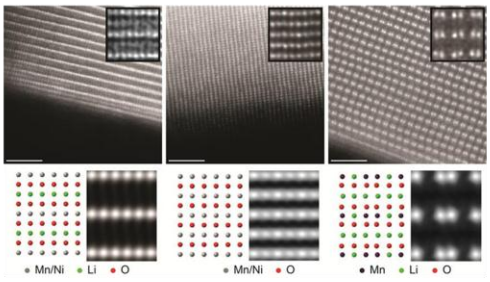
To implement these approaches, we have structured the EFRC:CST into two general thrust areas combining both experiments and theory. Thrust I, **Designing CST Materials and Interfaces,** aims to design, synthesize, and characterize materials and interfaces that we will use to reduce the complexity of nanostructured OPV and EES materials into unambiguous and well-characterized model systems. Thrust II, **Understanding CST Mechanisms,** aims to measure and simulate charge separation and transfer dynamics in model systems that span structural complexity from single molecules and single crystals to bulk heterojunctions.

Thrust I: Designing CST Materials and Interfaces:

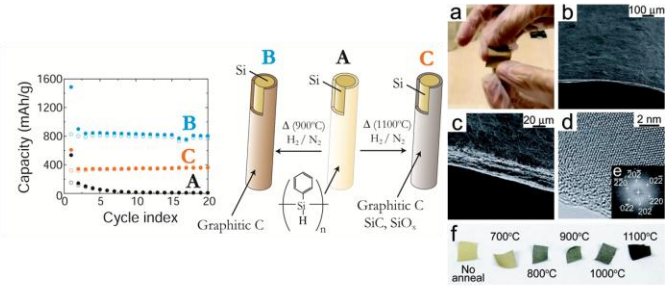
Single-chain, model OPV systems



OPV interfacial prototypes

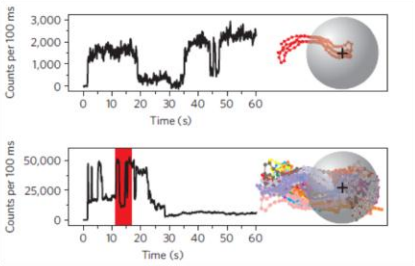


Li-ion battery materials with tunable morphology

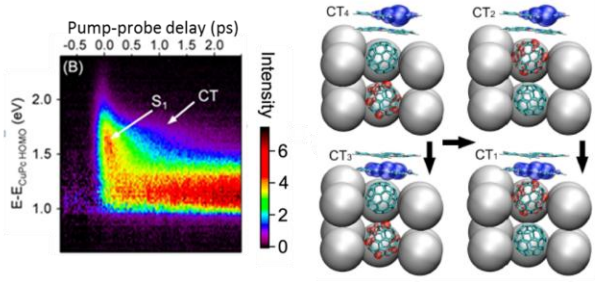


Lightweight, flexible Li-ion battery materials

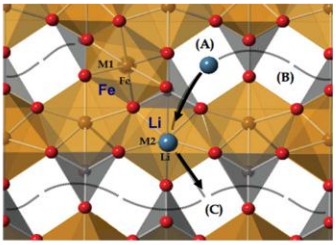
Thrust II: Understanding CST Mechanisms:



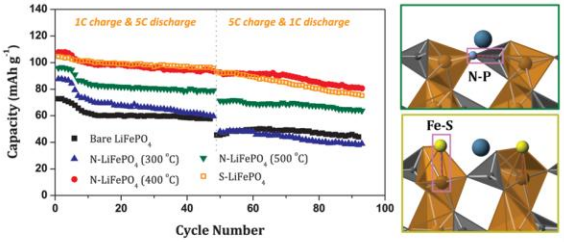
Long-range energy transfer in OPV polymer aggregates



Observation of OPV charge separation dynamics



Concerted Li+ diffusion around anti-site defects



Enhanced charge transfer by surface modification of $LiFePO_4$

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