Molecularly Engineered Energy Materials (MEEM)
EFRC Director: Vidvuds Ozolins
Lead Institution: University of California, Los Angeles

Mission Statement*: To acquire fundamental understanding and control of nanoscale materials for solar energy generation and electrical energy storage*.

MEEM will focus on materials that are inherently inexpensive (such as polymers, oxides, metal-organic frameworks), can be easily assembled from intelligently designed building blocks (molecules, nanoparticles, polymers), and have the potential to deliver transformative economic benefits in comparison with the current crystalline- and polycrystalline-based energy technologies. We will conduct systematic studies of the fundamental mechanisms of carrier generation, energy conversion, as well as transport and storage of charge and mass in tunable, architectonically complex materials. Fundamental understanding of these processes will enable rational design, efficient synthesis and effective deployment of novel three-dimensional material architectures for energy applications. MEEM will apply the center's unifying concept of controlling nanometer-scale architectures for achieving unprecedented device performance and manufacturing scalability to two research thrusts: solar energy generation and electrochemical energy storage. We expect to generate molecular design rules for production of optimized nanometer-scale architectures for high performing OPV devices and supercapacitors.

In solar energy conversion, organic photovoltaics (OPVs) offer unique and commercially attractive benefits of lower cost and large-area solution based processing. However, the performance of the most efficient OPV, Bulk Hetero Junction (BHJ) devices, suffers from unreliable synthesis techniques that heavily depend on processing kinetics. Polymer thin-film processing kinetics do not scale well from the laboratory to manufacturing settings, hence, there is a significant need for the rational design of materials that will form robust OPV architectures no matter how they are processed. MEEM will develop the ability to design molecules and architectures for OPV applications in an integrated effort spanning length scales from molecules to complete devices. The center effort involves a combination of self-assembly and molecular recognition with theory, synthesis, and characterization. Our aim is to gain a physical understanding of the architectures and molecular properties that control performance in OPVs, and to develop methods to robustly control those properties using molecular self-assembly. The goal is to engineer devices from the molecules up, optimizing structure and function through routes that will ultimately be better and more reliable than processing kinetics.

Highlights of our progress include demonstration of unique beneficial photophysical behaviors of OPV devices that directly results from designed molecular architecture via self-assembly: nm-scale amphiphilic polymer/fullerene co-assembilies. Our center's work in new fullerenes capable of molecular recognition also yielded a new ***design rule for fullerene acceptors: the optimal nanostructure for fullerene acceptors is an electrically connected linear structure***. The polymer self-assembly approach is a unique

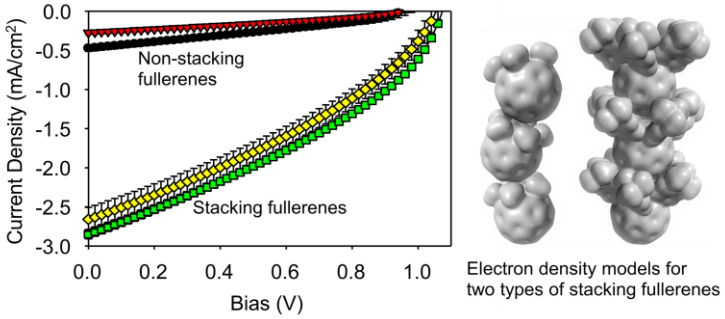

Figure 1. So-called "shuttlecock" molecules based on the heterofullerene $C_{59}N$ with phenyl "feathers" optimized for ideal close contacts within stacks. These molecules self-assemble into one-dimensional wires (right), enhancing the efficiency of charge separation and carrier transport in organic solar cells (left).

element of our center. Our future OPV efforts are focused on translating these assembly motifs into novel, robust, and high performing OPV device structures.

In energy storage, supercapacitors based on inexpensive metal oxides present an attractive option for large-scale storage from intermittent sources, such as wind and solar, but their widespread adoption is hampered by efficiencies that are significantly lower than theoretical estimates. Our hypothesis is that inefficient charge transport in bulk insulating materials is a crucial bottleneck. MEEM will apply our expertise in understanding and controlling nanometer-scale architectures to elucidate the microscopic factors that limit the performance of oxide-based electrochemical supercapacitors. We will design hierarchically structured electrode materials that integrate electronic and ionic conduction with pseudocapacitive charge storage. We will also search for new inexpensive materials that combine metallic conductivity with ability to capacitively store charge and explore the efficiency of these storage mechanisms in nanoporous materials using both theoretical and experimental approaches.

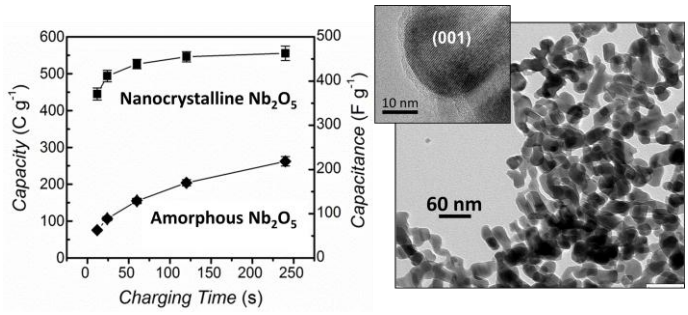

Figure 2: Electrochemical capacitors made from Nb_2O_5 nanocrystals yield significantly faster lithium ion charging kinetics compare to the amorphous form of the mesoporous film.

A notable achievement of our electrochemical supercapacitor team includes the discovery of fast lithium-ion charging kinetics in nanocrystal Nb_2O_5 capacitors, which yielded the highest capacitance observed with Nb_2O_5, at approximately 370 F/g in 12 seconds. The work also produces a ***design rule for Nb_2O_5 and mesoporous film based supercapacitors: presence of an ordered structure is important to achieve high capacity for the insertion reaction***. Additionally, an 3D numerical tool was developed and validated for predicting the capacitances of electric double layer capacitors (EDLCs), offering scaling laws for capacitance-voltage (CV) measurements in EDLCs, providing additional ***design rules for an optimum electrode architecture for ion transport***.

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University of California, Los Angeles	V. Ozolins (Director), B. N. Dunn (Assistant Director), Y. Lu, D. Neuhauser, L. Pilon, Y. Rubin, B. J. Schwartz, S. H. Tolbert
University of California, Berkeley	M. D. Asta
University of Kansas	B. Laird
National Renewable Energy Laboratory	N. Kopidakis
Eastern Washington University	Y. Hondonougbo
University of Washington	S. Jenekhe

Contact: Vidvuds Ozolins
Professor, Dept. of Materials Science & Engineering
vidvuds@ucla.edu
(310) 267-5538
http://meem.ucla.edu