Center for Mesoscale Transport Properties (m2m/t)
EFRC Director: Esther S. Takeuchi
Lead Institution: Stony Brook University
Class: 2014 – 2022

***Mission Statement**: To build the scientific knowledge base necessary to enable future creation of scalable electrochemical energy storage systems with high energy, high power, and long life.*

The research conducted under this award (m2m/t, molecular to mesoscale over time) will build the necessary insights to move beyond the flat electrodes in widespread use today to achieve the mission. In particular, it is imperative to understand and address transport limitations of multiple electrode architectures in electrochemical systems and their evolution over time. In order to achieve scalable electrochemical energy storage systems, facile ion transport and electron transfer are essential. The research conducted by the *m2m/t* Center will overcome current barriers resulting from existing knowledge gaps. The Center will pursue three Science Goals (SG) where each will be achieved through specific Research Objectives. The *Science Goals* (SG) are listed below where active material design is pursued in SG1 to facilitate transport and cycle life. SG2 addresses interface design and stability, to gain fundamental understanding of key considerations for multiple electrode designs. SG3 explores electrode architectures enabling ion access from the electrolyte to minimize transport losses in reaching all active material particles. The Science Goals represent interactive initiatives where SG1 and SG2 will ultimately enable the full realization of SG3 addressing the Center mission.

SG1. Design and create innovative multifunctional materials that synergistically integrate the multiple functions provided by individual components in battery electrodes.

SG2. Understand and control interfacial phenomena by deliberate design and manipulation of dynamic interfaces.

SG3. Gain fundamental understanding of design and function of thick porous electrode architectures.

Electrochemical function will be investigated with state-of- the-art tools, including *in-situ* and *operando* methods, where spatial and temporal resolution will be utilized to understand transport and transport limitations. Our focused and integrated effort with expertise in materials, theory, modeling and experimentation will deliver meaningful insights to benefit both current and next generation battery systems.

Approach: The *m2m/t* Center will achieve the goals via: 1) Synergistic interaction of experts in materials, characterization, theory, modeling, and electrochemical systems analysis; 2) Deployment of revolutionary analytical tools including electron microscopy and photon science with unprecedented resolution as well as real-time data acquisition capabilities; and 3) Investigation unified by innovative material concepts and versatile electrode constructs.

Under Science Goal 1 the research will probe several critical science questions. Can multifunctional materials be successfully designed and synthesized? How do electronic conductivities compare to the native oxides? Will integrating multiple functionalities into these materials result in enhanced electrochemical transport properties in electrochemical energy storage devices? Can electrochemical cycle stability be enhanced through purposeful material design and manipulation?

Under Science Goal 2 the research will pursue the following questions. Will deliberately designed and synthesized model electrode structures enable interface composition, properties, and time-dependent evolution to be interrogated using high signal-to-noise bulk measurements? Will advanced analytical approaches allow characterization of dynamic interfaces of electrochemical energy storage systems? Using insights from multiscale modeling, theory, and experiment, can interfacial phases with specific chemical composition be created for use in model electrochemical systems suitable for quantitative comparisons and refinement of multiscale models?

The activities under Science Goal 3 will investigate the following questions. Can targeted design of 3D electrode architectures overcome ion transport limitations to enable high power and high capacity scalable designs? Will exploitation of state-of-the-art in-situ and operando methodologies to characterize materials properties and electrode dynamics under realistic operating conditions provide sufficient spatio-temporal resolution to develop continuum models? Will integration of existing and new computational techniques adequately predict temporal evolution of spatially distributed properties to advance next generation energy storage?

The Center is pursuing these critical issues to move beyond conventional electrode architectures based on flat 2D layers where active materials interact through short distances and over large lateral areas. The proposed research tackles fundamental limitations of incomplete active materials reaction and sluggish transport kinetics through considering the multiple length scales critical to electrode design and function, **Figure 1**. The Center research will advance function-oriented electrode design *via* integrated experimental and theoretical approaches, including rational material design, structural engineering through novel synthesis, interface stabilization and advanced *ex-situ*, *in-situ*, and *operando* characterization tools linked with comprehensive theory and continuum modeling. This integrated effort will empower the community to move from serendipitous trial and error to rational design, and from compartmentalized knowledge to integrated understanding.

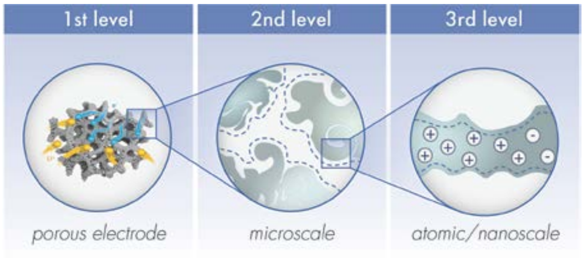

Figure 1. Multiscale transport in electrode architectures.

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