EFRC: CENTER FOR MESOSCALE TRANSPORT PROPERTIES (*m2m*)

UPDATED: OCTOBER 2016

AWARDS: \$10.4M (August 2014 – July 2018)	
WEBSITES: http://science.energy.gov/bes/efrc/centers/EFRC/; http://www.stonybrook.edu/m2m	
TEAM: **Stony Brook University (Lead):** Esther S. Takeuchi (Director), Amy C. Marschilok (Center Operations Officer), Maria Fernandez-Serra, Kenneth Takeuchi, Stanislaus Wong; **Brookhaven National Laboratory**: Hong Gan, Mark Hybertsen, Ping Liu, Eric Stach, Feng Wang, Jun Wang, Yimei Zhu; **Columbia University**: Alan West; **Georgia Institute of Technology**: Elsa Reichmanis; **University of North Carolina:** Joseph DeSimone; **University of California at Berkeley:** Nitash Balsara; **Oak Ridge National Laboratory:** Nancy Dudney**; Rensselaer Polytechnic Institute:** Robert Hull; **University of Texas at Austin:** Guihua Yu	

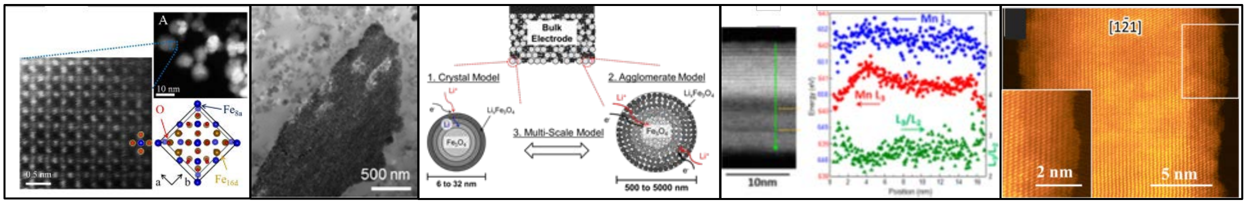
SCIENTIFIC MISSION AND APPROACH

The mission of the Center is to understand and provide control of transport properties in complex battery systems with respect to multiple length scales, from molecular to mesoscale (*m2m*); to minimize heat and maximize work of electrical energy storage devices. While battery inefficiency can be approached at the macro level, emphasizing bulk parameters and bulk methods cannot fully interrogate or address the inherent heterogeneity of ion and electron flux contributing to the local resistance within an electrode and at the interfaces. In order to develop the capability to predict and ultimately control energy storage systems, these inefficiencies must be understood not just as a bulk property (heat), but rather as localized resistance at the molecular to mesoscale (*m2m*) levels. The center has three Scientific Inquiry Areas (SIA):

1. **What are the *fundamental limits* of ion and electron transport and electron transfer over multiple length scales?** Investigation of transport and transfer phenomena for redox active moieties with several configurations and considering the roles of structure, crystallite size and particle size.
2. **How do the phenomena change across *multiple domains* including interfaces?** The influence of physical properties, surface functionalization, and process on the transfer and transport properties and the function of composite electrodes will be explored.
3. **How do the transport phenomena evolve *over time* in systems not at equilibrium?** The effect of extended cycling on energy related solids will be studied to determine the effect of time.

SELECTED SCIENTIFIC ACCOMPLISHMENTS

- A comprehensive investigation of multi-electron transfer reactions in Fe_3O_4 was conducted using experiment and *ab-initio* calculations. Results provide the 1st experimental evidence that the cubic-close-packed (ccp) O-anion array in Fe_3O_4 is sustained throughout lithiation and delithiation.
- Detailed analysis of composite electrodes formulated using nanocrystalline Fe_3O_4 quantified the presence of active material aggregates. The first multi-scale mathematical model accounting for mass transport on both the crystal and agglomerate length-scales was developed for magnetite electrodes. Active material utilization predictions due to transport limitations on the material and aggregate size were made possible.
- First direct experimental demonstration of lateral (ab plane) Li^+ diffusion in 1D α-MnO_2 type materials. Identified possible link with surface oxygen vacancies.
- The formation of a conductive network through a reduction-displacement reaction in $Ag_xV_yPO_4$ type materials was mapped via EDXRD. The data revealed that a composite electrode formulation is beneficial, but does not ensure complete electrical contact of each active particle.



m2M research, from left: Annual dark-field (ADF) image of a Fe_3O_4 nanoparticles with high-angle ADF image and structural model; Nanocrystalline Fe_3O_4 aggregate TEM image; First predictive multiscale continuum model; STEM-HAADF image of $Ag_{1.16}Mn_8O_{16}$ nanorod. EELS results indicating surface oxygen vacancies; Regenerated α-MnO_2 nanofiber after 100 cycles.

IMPACT

- *m2m* EFRC organized a one-day workshop on Advanced Characterization Techniques for Energy Storage jointly hosted by BNL's Center for Functional Nanomaterials (CFN) and National Synchrotron Light Source-II (NSLS-II). Attendance included other energy storage EFRCs and JCSER. Participated in the Electrochemical Energy Summit at the 228th Electrochemical Society.
- Impact of *m2m* Center noted through 9 invited talks and 5 invited publications including the following. Keynote address at the National Academy of Inventors Induction ceremony in Pasadena, CA. Invited presentation on Contemporary Issues and Case Studies in Electrochemical Innovation 2 at PRIME. Held every four years, this international gathering is the joint effort of The Electrochemical Society (ECS), The Electrochemical Society of Japan (ECSJ), and The Korean Electrochemical Society (KECS).
- *m2m* Director co-authored an invited "Best Practices for Reporting on Energy Storage" editorial for ACS Applied Materials and Interfaces.
- NY state matching funds for the *m2m* EFRC award were obtained to establish a new pouch cell facility for assembly of prototype batteries in the dry room at BNL. This will provide a new institutional resource as a result of the EFRC project.
- *m2m* investigations on Ag^+ and Ag^0 contributions to conductivity led to conceptualization of new program on solid state electrolytes funded by EERE for $1.2M.

PUBLICATIONS AND INTELLECTUAL PROPERTY

As of Oct 2016, *m2m* had published 33 peer-reviewed publications cited over 100 times, filed 2 disclosures and 2 US patent applications. The following is a selection of impactful papers:

- Abraham, A., Housel, L. M., Lininger, C. N., Bock, D. C., Jou, J., Wang, F., West, A. C., Marschilok, A. C., Takeuchi, K. J. & Takeuchi, E. S. Investigating the Complex Chemistry of Functional Energy Storage Systems: The Need for an Integrative, Multiscale (Molecular to Mesoscale) Perspective. *ACS Central Science* **2,** 380-387, doi: 10.1021/acscentsci.6b00100 (2016). Invited. [**1 citations**].
- Dudney, N. J. & Li, J. Using all energy in a battery. *Science* **347,** 131-132, doi: 10.1126/science.aaa2870 (2015). [**19 citations**].
- Zhang, W., Bock, D. C., Pelliccione, C. J., Li, Y., Wu, L., Zhu, Y., Marschilok, A. C., Takeuchi, E. S., Takeuchi, K. J. & Wang, F. Insights into Ionic Transport and Structural Changes in Magnetite during Multiple-Electron Transfer Reactions. *Advanced Energy Materials* **6,** 1502471, doi: 10.1002/aenm.201502471 (2016). [**3 citations**].
- Wu, L., Xu, F., Zhu, Y. *et al*. Structural defects of silver hollandite, $Ag_xMn_8O_y$, Nanorods: Dramatic impact on electrochemistry. *ACS Nano* **9**, 8430-8439, doi: 10.1021/acsnano.5b03274 (2015). [**10 citations**].
- Poyraz, A., Huang, J., Cheng, S. *et al.* Effective Recycling of Manganese Oxide Cathodes for Lithium Based Batteries. *Green Chem*. **18,** 3414-3421, doi: 10.1039/C6GC00438E (2016). [**0 citations**]
- Bock, D., Pelliccione, C. J., Zhang, W. *et al*. Dispersion of Nanocrystalline Fe_3O_4 Within Composite Electrodes: Insights on Battery Related Electrochemistry, *ACS Appl. Mater. Interfaces* **8,** 11418–11430, doi: 10.1021/acsami.6b01134 (2016). [**4 citations**].