Nanostructures for Electrical Energy Storage (NEES)
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Lead Institution: University of Maryland
Class: 2009 – 2020

Mission Statement*: To reveal scientific insights and design principles that enable a next-generation electrical energy storage technology based on dense mesoscale architectures of multifunctional solid state nanostructures.*

In its first phase (2009-2014) NEES research was aimed at the design and electrochemistry of individual heterogeneous, multifunctional nanostructures as a pathway to high power energy storage together with stability during charge/discharge cycling. In its second phase (2014-2018) NEES-2 concentrated on architectural design, i.e. how to arrange precision nanostructures into dense mesoscale architectures for the same goals and to explore the new mesoscale science that emerges. In its current third phase, NEES-3 is focusing its full attention on all-solid-state electrochemical storage.

The opportunities in solid state storage (batteries and capacitors) are profound. Research on solid electrolytes and their electrode interfaces is miniscule compared to liquid-electrolyte systems, posing profound scientific challenges to understand the roles of chemical and electrostatic interactions at these interfaces. Advanced synthesis techniques from NEES play an enlarged role in solid state, enabling novel architectures that promise significant performance advantages and expanding potential applications beyond transportation and grid to biomedical, internet-of-things, and information storage for analog computation (Figures 1-3).

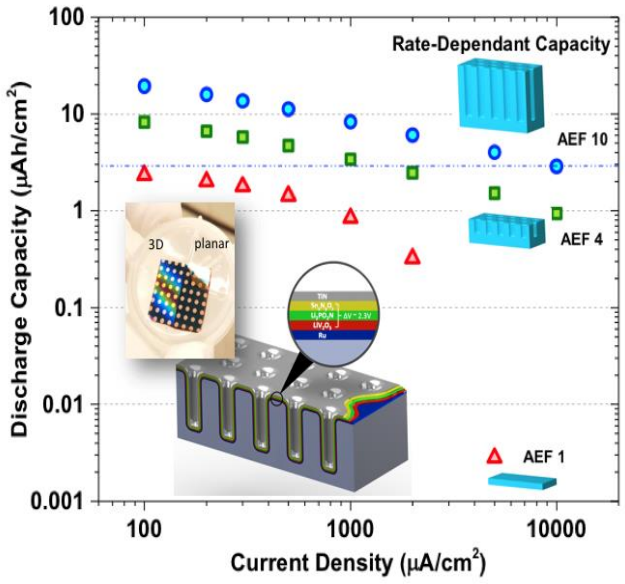

Figure 1. 3-D solid state battery enhances power and energy, shown here in comparison to planar (AEF 1) configurations.

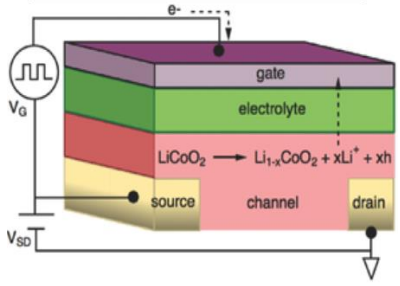

Figure 2. Solid state battery inspires nonvolatile redox memory based on ions stored in electrode

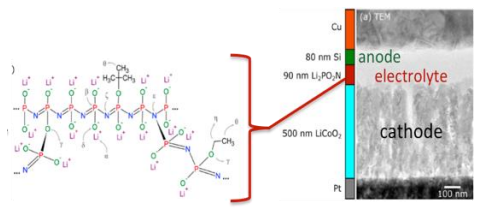

Figure 3. Highly controlled thin film synthesis (here ALD LiPON solid electrolyte) enables diverse 3-D architectures.

Many of the critical science questions are centered at interfaces, particularly that between solid electrolytes and electrodes, driving both theoretical efforts in computation (Figures 4-5) and experimental work in scanning probe microscopies and particularly for operando observations (Figures 6-7). Theoretical efforts are pursued at multiple length scales. Molecular-level DFT calculations reveal reaction energy barriers and likely kinetics. Continuum mechanics shows the changes in material properties induced by

volume changes as ions are transported back and forth between electrode materials. Molecular dynamics provides insight into stochastic distributions that can dominate degradation and failure.

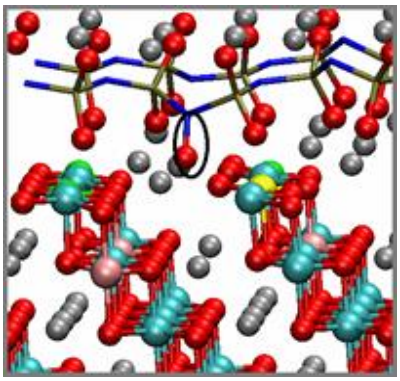

Figure 4. Model LiPON solid electrolyte is oxidized by $LiCoO_2$ cathode.

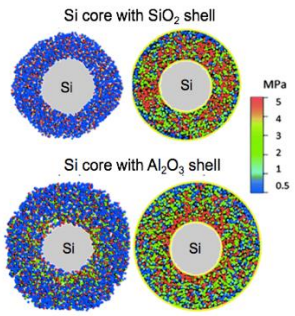

Figure 5. Stress evolution with lithiation/delithiation off core-shell nanostructures.

Experimental efforts are particularly aimed at understanding the complex energy landscape of critical regions in ionic solid state systems, specifically recognizing that the ions react according to chemical potentials but are sensitive to electrostatic (voltage) potentials during transport, while the reactions in which ions engage transform voltage contours across and near heterogeneous interfaces. Access to these and related issues is enabled by novel characterization approaches, including cross-sectional sample arrangements, patterned synthesis of multilayer structures, and localized electrochemical and mechanical configurations probed by operando SPM techniques.

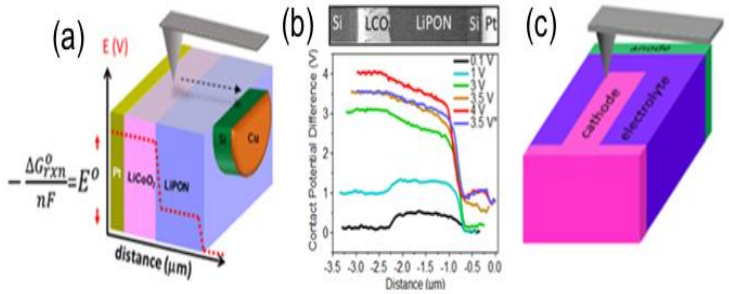

Figure 6. (a,b) KPFM voltage profile across solid interfaces; (c) KPFM operando imaging in 3D interdigitated solid state battery.

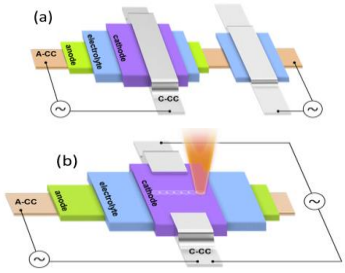

Figure 7. Patterned thin film testbeds to characterize solid state battery electrochemistry (a) and to identify specific energy barriers at interfaces as a function of charge state.

The potential scientific impact in fundamental understanding of all-solid-state electrochemical storage is profound, attracting a growing community of researchers, with important and diverse applications in sight. NEES looks forward to expanding its current leadership in this research domain.

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