Nanostructures for Electrical Energy Storage (NEES)
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Lead Institution: University of Maryland
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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 nanostructures.*

In its first phase (2009-2014) NEES focused on the design and electrochemistry of heterogeneous, multifunctional nanostructures as the building block for electrical energy storage (EES) configurations offering high power and stability during charge/discharge cycling. Using prototype materials relevant to Li ion batteries, NEES has employed both novel single-nanostructure platforms and "forests" of densely packed nanostructure arrays to fuel insights into nanostructure electrochemistry.

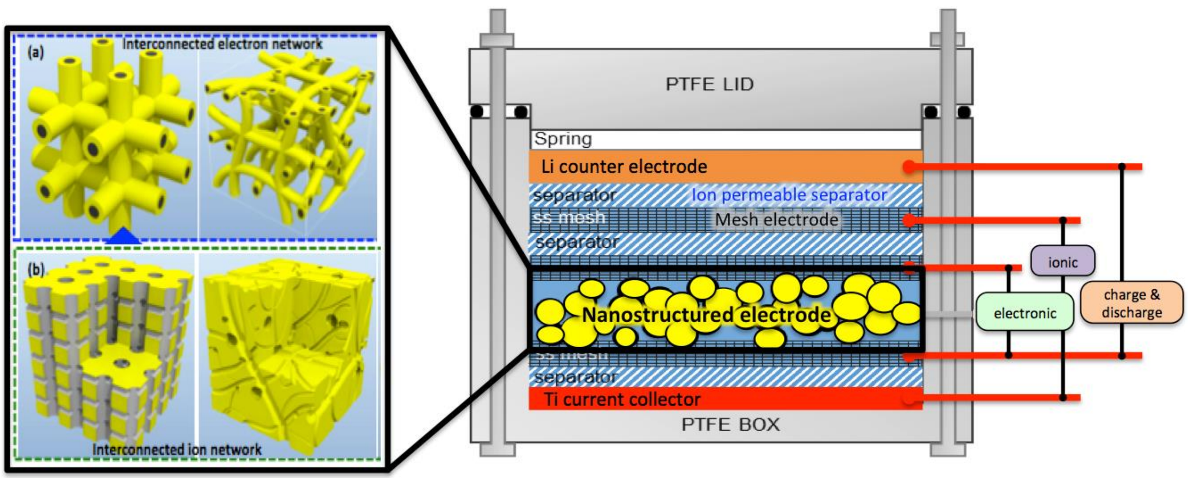

Figure 1. Mesoscale architectures of nanostructured electrodes, compared by *In-operando* ionic & electronic conductivity measurements as a function of charge state (degree of lithiation) and charge/discharge cycles.

In its second phase (2014-2018) NEES is concentrating on the arrangement of precision nanostructures into dense mesoscale architectures and the new scientific challenges that result. These investigations begin with achievable architectures (Fig. 1), which raise questions such as: What 3-D synthesis strategies translate the benefits of precision nanostructures to dense mesoscale assemblies? How does the EES behavior of regular/ordered architectures compare with that of pseudorandom counterparts? How well do metrics for the latter, such as porosity and tortuosity, forecast EES performance? The dense packing of nanostructures into mesoscale architectures raises new questions about ion and electron transport in confined nanogeometries, e.g.: Will electrolyte nanoenvironments contain and supply ions in sufficient concentration to fully utilize EES storage layers in the nanostructures? What design guidelines are needed to balance electron and ion transport (in current collectors and electrolyte respectively) to achieve high power? Will surface charge vary along nanostructures, and what role might it play in electrolyte ion transport phenomena (e.g. electrokinetics)? Comparisons between the diverse electrode architectures developed in NEES are being compared using a new configuration that enables separate determination of ion and electron transport kinetics and conductivity.

NEES also seeks to understand capacity degradation and failure in nanostructure-based EES - an ambitious effort to establish a science of nanostructure degradation, simultaneous with or in advance of a prototype nanostructure-based EES technology. NEES is using advanced nano/micro scale platforms (Fig. 2) to identify degradation/failure in both early (<10's of cycles) and extended-term (~50-1000 cycles) charge/discharge cycling, from which follow-on experiments can address validation of proposed degradation. Test structures can be constructed and tested to validate proposed degradation mechanisms.

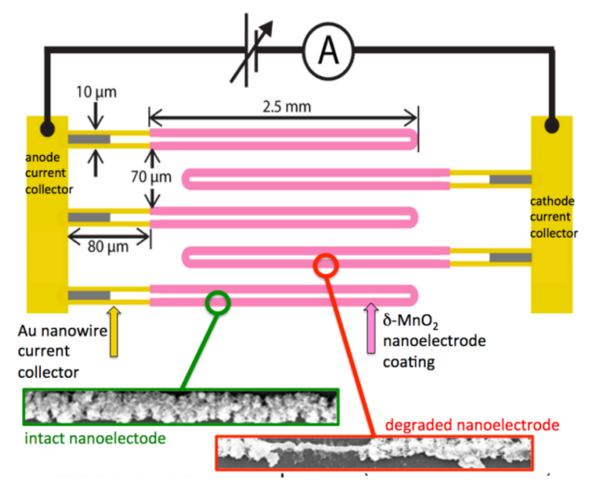

Figure 2. Long nanoelectrodes as testbeds for nanobattery degradation and failure mechanisms.

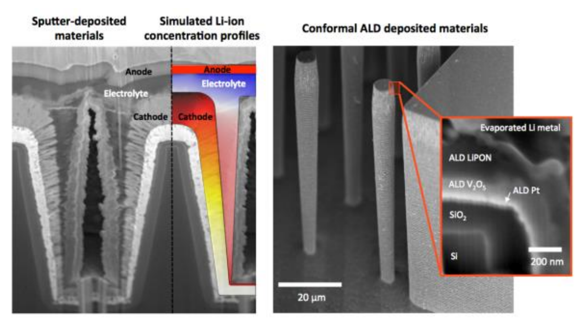

Figure 3. 3D solid-state batteries using different synthesis techniques, with multiphysics model of Li transport.

As an ambitious alternative for safe, high performance EES, NEES is working on solid electrolyte materials and synthesis of interdigitated 3-D structures for solid state nano/micro batteries (Fig. 3), closely coupled with multiphysics modeling. Synthesis techniques play a strong role here in enabling viable 3-D configurations. Solid electrolyte layers are particularly central to success, not only in solid state batteries but also to serve as ion-conducting passivation/protection layers for exploiting the high energy density of metal anodes in other battery systems.

These directions build on NEES expertise in the science of electrochemical interfaces, pioneering nanocharacterization methods, and a portfolio of modeling and simulation techniques from molecular to micro/macro scale. NEES research is addressing a variety of advanced battery chemistries as well as Li ion, involving metal anodes, multivalent ions, sulfur and oxygen cathodes, employing controlled materials and nanostructures to understand, assess and improve EES behavior.

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