

Synthetic Control Across Length-scales for Advancing Rechargeables (SCALAR)

EFRC Director: Sarah Tolbert

Lead Institution: University of California, Los Angeles

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Mission Statement: *To use the power of synthetic materials chemistry to design materials, interfaces, and architectures that help solve long-standing problems in electrochemical energy storage.*

Lithium-ion batteries have dominated rechargeable electrical energy storage for over two decades. Fundamentally, however, materials for lithium-ion batteries have changed little during this time, even though both their applications and desired performance have expanded tremendously. The scientific mission of the SCALAR EFRC is based on leveraging the power of modern materials synthesis and characterization to create and understand, at a fundamental level, a new generation of battery materials that can overcome many of the limitations intrinsic to the archetypal intercalation hosts in use today. Within the SCALAR EFRC, the challenge we face is to rethink the chemistry associated with secondary ion batteries to dramatically expand the range of materials and chemistries that can be employed, to increase stability by controlling transport, and to control architectures and interfaces to enable the use of very high capacity materials.

The overarching center goal is to combine cutting edge synthetic methodologies with a multi-length scale view of energy storage to make non-incremental improvement in battery materials. From a broad perspective, our program seeks to:

1. Take a holistic approach to the design of new functional materials that bridges the atomistic, nanometer, and macro length-scales in the quest to improve battery performance
2. Leverage molecular and solid-state synthetic methods, combined with solution phase self-assembly, to create new electrode materials that increase capacity, reduce losses, and improve reversibility in rechargeable batteries

To address its mission, the SCALAR EFRC has defined five scientific objectives that represent particularly promising routes for achieving its goals. As a center, we aim to:

1. Synthesize new electrode materials that increase charge storage capacity by integrating the electrochemistry of anions and cations into a single material.
2. Reduce resistive losses in electrodes using doping to create conductive electrode materials and conductive binders and scaffolds to increase conductivity in composite electrodes.
3. Create nanoscale architectures and interfaces that improve reversibility by stabilizing electrodes against chemical degradation, facilitating desired reactions, and accommodating the morphological changes that occur upon cycling.
4. Design systems to optimize charge transfer processes across length-scales, from the atomic, to the particle, and finally to the electrode level.
5. Integrate molecular, solid-state, and self-assembly methods to create structures that achieve nanoscale control and atomic-scale precision in macroscopic architectures.

The center is organized in to three thrusts. Thrust 1, aimed at objective 1, uses a combination of anion cluster chemistry, anion intercalation chemistry, and anion redox in extended inorganic solids to integrate anion redox with cation redox in new materials. Thrust 2 attacks the problem of resistive losses outlined

in objective 2 in two very different ways – first by exploring the use of conjugated polymers as binders with increased electrical and ionic conductivity, and second by exploring highly covalent and shear structures with enhanced ionic and electrical conductivity. These efforts are coupled with electrochemical calorimetry to directly measure thermal loss within our systems. Finally, Thrust 3 aims to solve the challenge of objective 3 by using inorganic surface coatings for improved stability and reversibility, using flexible nanoporous architectures that can mitigate and even compensate for large volume changes during cycling, and using catalysts that can favor desired electrochemical reactions and mitigate unfavorable ones.

Thrust level objectives (1-3) are combined with two cross-cutting objectives (4-5) focused on utilizing a diverse range of synthetic methodologies and a multi-length scale view of battery materials to design new materials that can be optimally integrated into battery electrodes. In carrying out the research mission, materials synthesis and design considerations are combined with cutting edge materials characterization and high level predictive modeling to create true synergy in materials design, atomistic materials synthesis, mesoscale structural control, and materials characterization across length-scales. By taking a holistic view of energy storage, the SCALAR EFRC will expand the understanding of battery materials and have a long term impact on how we think about the kinds of new materials and reactions that can be utilized for rechargeable electrical energy storage.

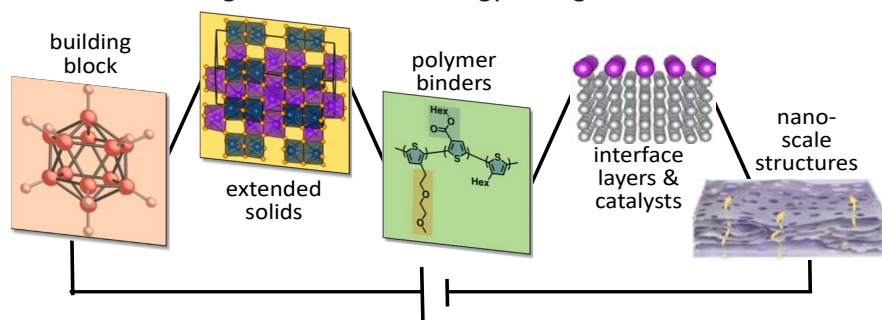


Figure 1: The SCALAR EFRC aims to rethink battery materials, starting from the level of building blocks and then moving to new motifs for extended solids. New materials are integrated with multifunctional polymer binders, designer interfaces, and controlled nanoscale architecture.

Beyond scientific synergy, the SCALAR EFRC takes advantage of the human synergy of the Southern California regional area, which houses a large number of world class research universities. Five of these universities, along with one California based national lab, have joined together to make the SCALAR center a regional hub for battery research that optimally leverages both the proximity and complementary facilities of the participating partner institutions.

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University of California, Los Angeles	Sarah Tolbert (Director), Bruce Dunn (Deputy Director), Xuan Duan (Thrust 3 Lead), Laurent Pilon, Philip Sautet, Alexander Spokoyny
University of California, Santa Barbara	Ram Seshadri (Thrust 2 Lead), Bradley Chmelka, Rachel Segalman, Anton Van der Ven
University of Southern California	Brent Melot (Thrust 1 Lead), Sri Narayan, Barry Thompson
Caltech	Tom Miller, Kimberly See
Stanford Synchrotron Radiation Lightsource	Joanna Nelson Weker
University of California, San Diego	Jian Luo

Contact: Sarah Tolbert, Director, tolbert@chem.ucla.edu
(310) 206-4767, www.chem.ucla.edu/SCALAR/