

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 this mission, the SCALAR-EFRC has defined five scientific objectives that we feel represent particularly promising routes to these goals. As a center, we aim to:

- 1) The overarching center goal is to take a multiscale view of materials design and fabrication, using diverse synthetic methods to optimize battery materials from the micro- to the macro-scale.
- 2) Thrust I specifically aims to improve energy density through the development of insertion hosts that show reversible multi-electron redox.
- 3) Thrust II focuses on improving power density by facilitating ion and electron transport using both atomistic and architectural optimization.
- 4) Thrust III takes on the challenge of improving reversibility through the optimization of bulk and interfacial structures, focusing on the intertwined goal of improving both chemical and mechanical stability.
- 5) A holistic view of all these efforts can be found in the overarching goal of reducing hysteresis in all aspects of electrochemical energy storage.

Within these goals, Thrust 1 aims to increase electrode capacity using a combination of anion intercalation chemistry, mixed anion and cation redox in extended inorganic solids, and two electron cation redox. Thrust 2 attacks the problem of improving power density by facilitating both electron and ion mobility in

battery materials. This thus effort combines conjugated polymers as binders with increased electrical and ionic conductivity, high ionic mobility phases, intrinsically conductive electrode materials, and nanoscale architectures. These efforts are coupled with electrochemical calorimetry to directly measure thermal loss within our systems. Finally, Thrust 3 aims to solve the challenge materials stability using inorganic surface coatings for improved stability and reversibility, flexible nanoporous architectures that can mitigate and even compensate for large volume changes during cycling, and catalysts that can favor desired electrochemical reactions and mitigate unfavorable ones.

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 our understanding of battery materials and have long term impact on how we think about the kinds of new materials and reactions that can be utilized for rechargeable electrical energy storage.

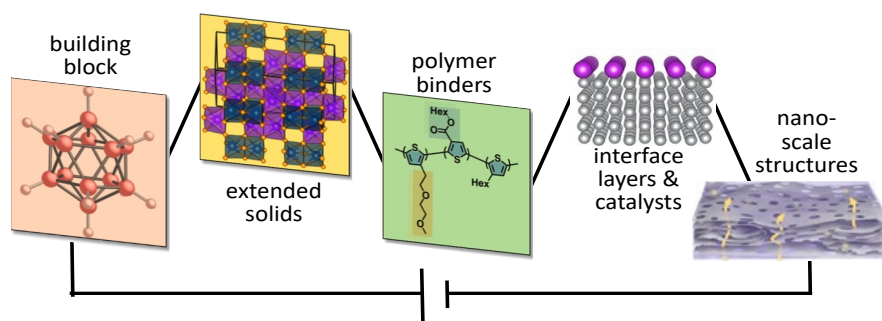


Figure 1: The SCALAR EFRC aims to rethink battery materials, starting from the level of building blocks and then moving to new motifs for extended solids. New materials are integrated with multifunctional polymer binders, designer interfaces, and controlled nanoscale architecture.

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 (Assistant Director), Xuan Duan (Thrust 3 Lead), Laurent Pilon, Philip Sautet
University of California, Santa Barbara	Ram Seshadri (Thrust 2 Lead), Bradley Chmelka, Anton Van der Ven
University of Southern California	Brent Melot (Thrust 1 Lead), Sri Narayan, Barry Thompson
Caltech	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/