Advancing Energy Storage: The Role of Petascale Computing

Presented to

Scientific Impacts and Opportunities in Computing

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Meeting world energy needs will require efficient electrical energy storage

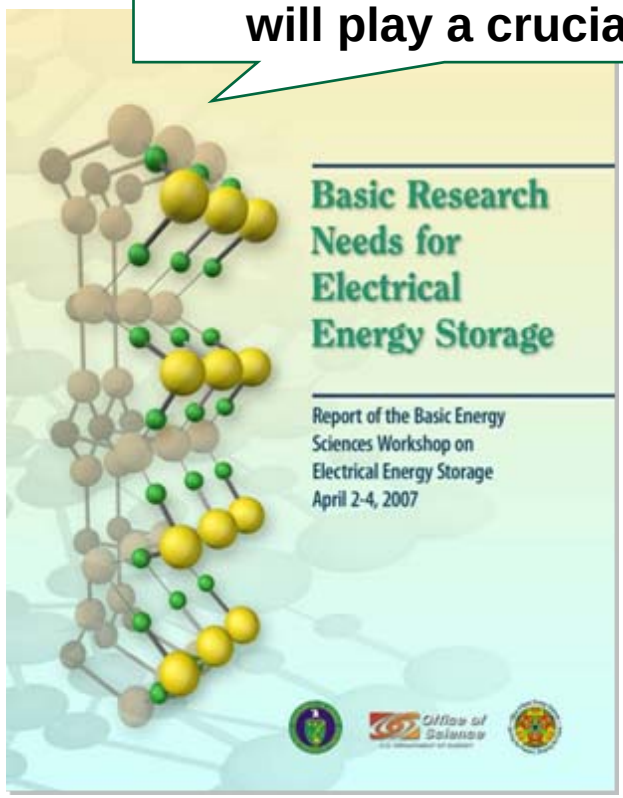
- **Today's electrical energy storage (EES) technologies fall far short of requirements for efficient use of electrical energy**
- **Revolutionary improvements are needed**
  - **To level the cyclic nature of intermittent renewable sources**
  - **To progress from today's hybrid electric vehicles to plug-in hybrids or all-electric vehicles**
  - **To enhance safety and reliability**

- **This will require transformational advances in the underpinning of materials and chemical sciences**
  - **Significant advances in the fundamental understanding of nanoscale phenomena**
  - **Predictive modeling of complex, multi-component systems over multiple length and time scales**

Basic Energy Sciences workshop:
Establishing a scientific foundation for technology breakthroughs

- **Theory, modeling, and simulation complement experimental efforts**
  - **Insight into novel charge storage mechanisms**
  - **Prediction of trends**
  - **Design criteria for new materials**
  - **Guidance for experiments**
  - **Ability to address a broader range of materials systems and compositions**
- **Large multiscale computations can provide fundamental understanding of processes**
  - **Phase transitions in electrode materials**
  - **Ion transport in electrolytes**
  - **Charge transfer at interfaces**
  - **Electronic transport in materials**
  - **Evaluation of complex systems**

"New computational methods will play a crucial role"



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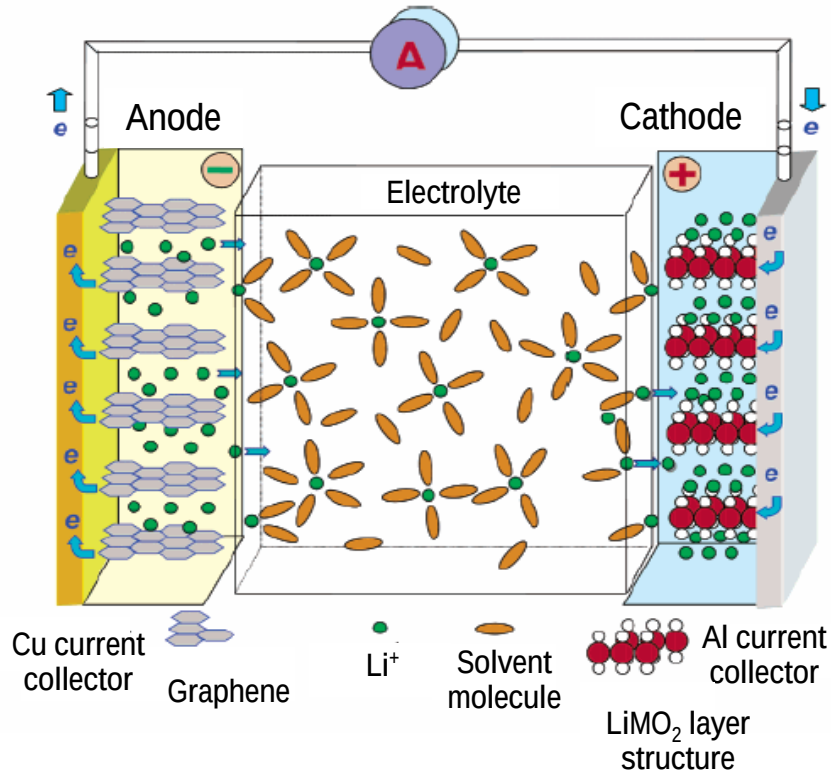
Chemical energy storage science

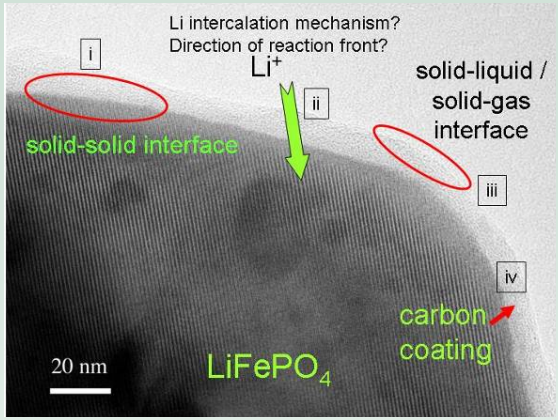


- **Store more energy per unit volume**
- **Tolerate thousands of charge/discharge cycles**
- **Long lifetimes**
- **Safety**
- **Low cost**
- **Need a factor of >3 in energy density and 100 in recharge time**

- **Batteries are dynamic systems that change with every charge/discharge cycle**
- **The apparently simple interface between electrode and electrolyte is in fact a complex set of phases that change with time**

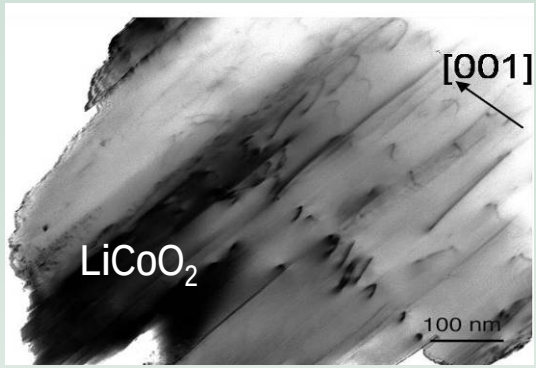
Chemical energy storage science: Fundamental challenges

Knowledge gap: **Basic understanding of the mechanisms and kinetics of the elementary steps involved in chemical storage**



How to correlate interface structure with reactivity?

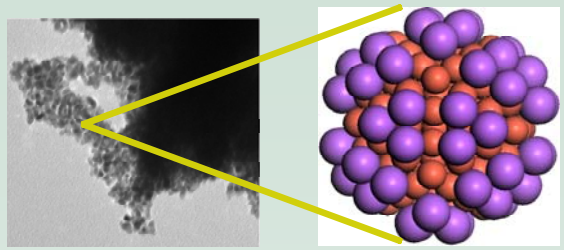
Need molecular-level understanding of ion intercalation or reaction at solid-liquid or gas-solid interface



How do structural defects, such as dislocations, change during cycling?

What is their relationship to fracture formation/ prevention?

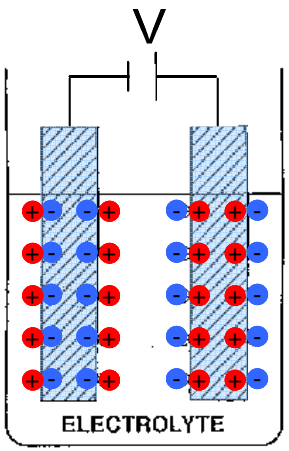
H. Gabrisch, R. Yazami, B. Fultz, Electrochem. Solid St. Lett. 5 (6), A111–A114 (2002)



To what extent do thermodynamics and kinetics of ion reactions differ between nano and bulk?

Novel ideas needed to handle nanoscale relevant to technology (10–150 nm)

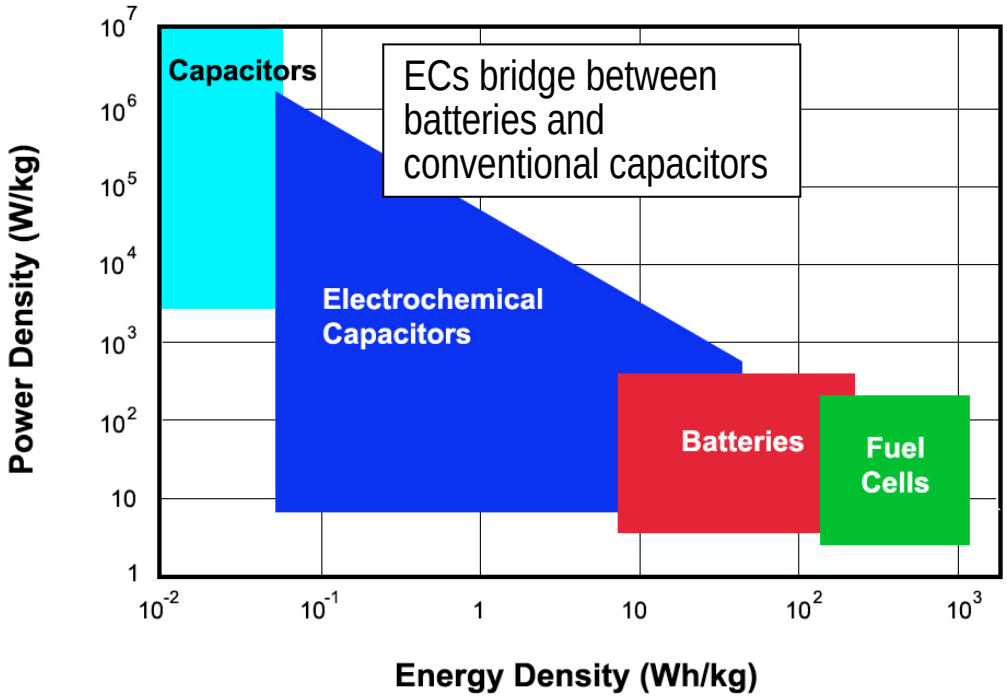
Capacitive storage science



Electrochemical double-layer capacitor (EDLC)

- EDLC: 2 carbon electrodes
- Pseudocapacitor: 1 carbon electrode, 1 battery-like electrode
- Store energy as charge, no chemical reactions, fast charge/discharge cycle, sub-second response time
- High power density, but need a factor of one hundred in energy density
- Versatile solutions for harvesting and regenerating energy

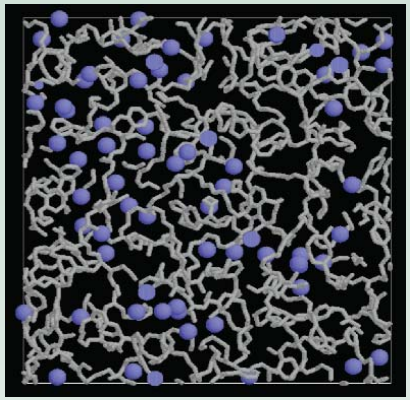
Adapted from M.S. Halpe and J.C. Ellenbogen, MITRE Nanosystems Group, 2006



- Fundamental understanding of electrochemical capacitors (ECs) still rudimentary
- Advances will require:
  - Understanding of charge storage mechanisms
  - Tailored multifunctional materials
  - New electrolytes

Capacitive storage science: Fundamental challenges

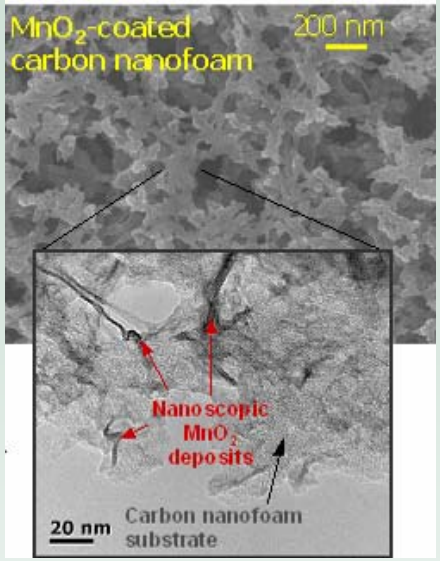
Knowledge gap: **Basic understanding of key issues involving interfaces, dynamics, and charging**



Reverse Monte Carlo simulations to understand relationship between pore size and interacting species

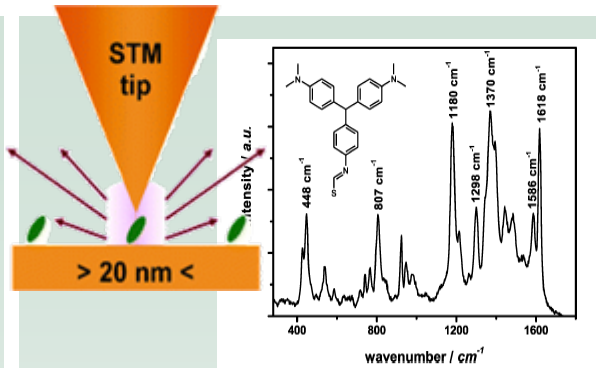
What is the equilibrium structure of ions and solvent in confined geometry?

How would pore size, surface area, and surface chemistry or functional group affect capacitive storage?



Multifunctional nano-architectures to enable:

- Ionic and electronic conductivity
- Facile permeation of electrolyte
- Effective charge storage functionality

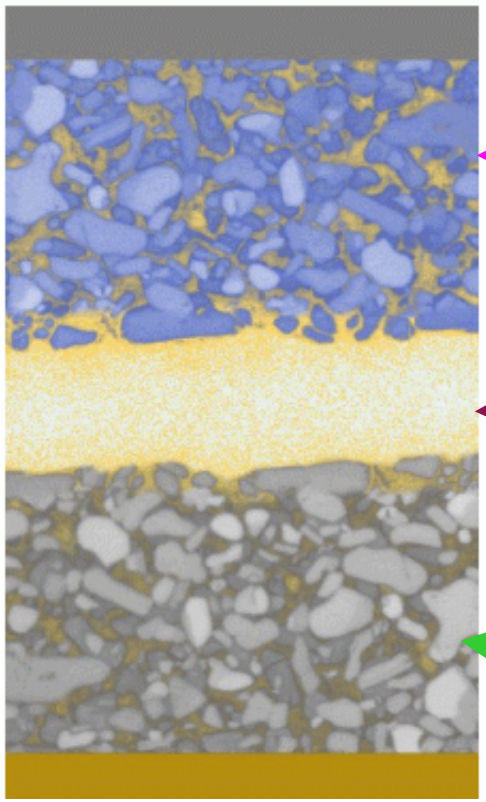


In situ tools to characterize electrode-electrolyte interface during charging/discharging

Develop and implement techniques to monitor

- Spatial resolution from atomic to mesoscopic
- Temporal resolution down to femtoseconds
- Changes in structure and composition

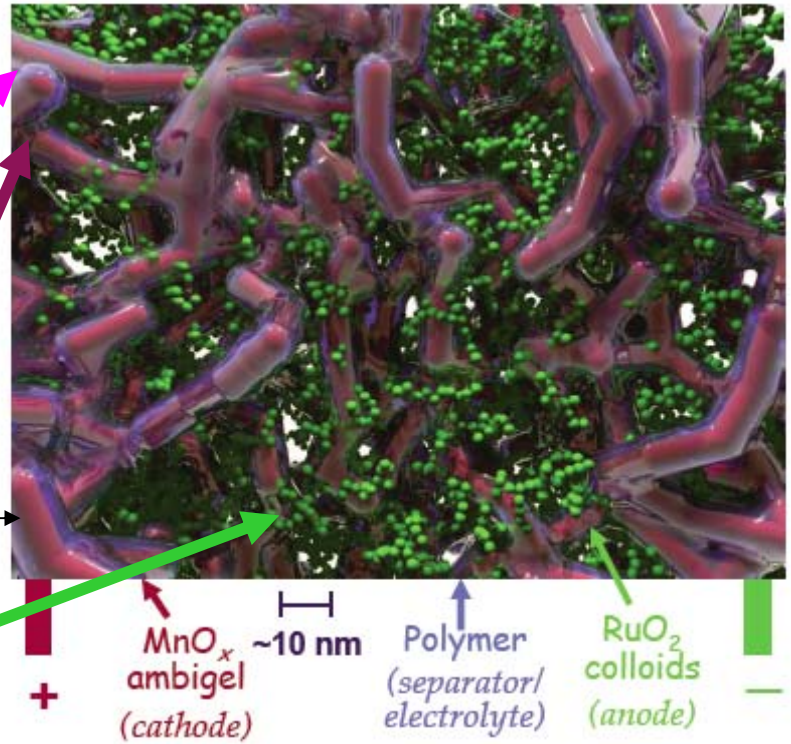
Chemical energy storage: Novel designs and strategies



Positive electrode

Electrolyte/separator

Negative electrode



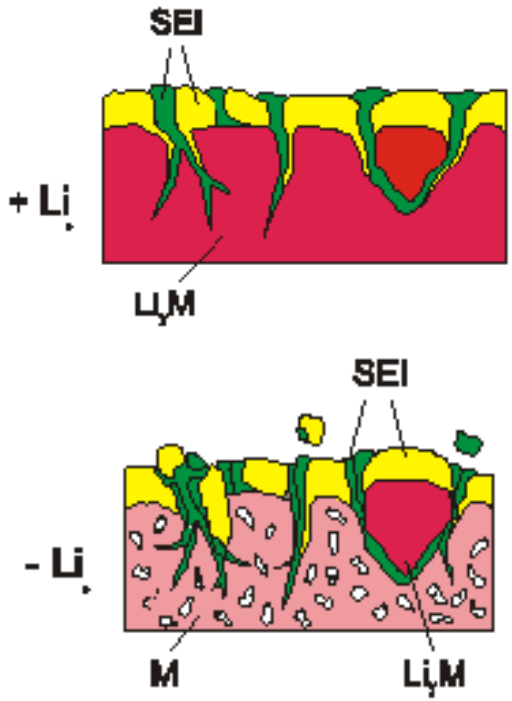
Present-day electrochemical cell structure

3-D battery: Self-assembled electrochemical cell structures containing multifunctional components

Courtesy of H. Feil, Philips Research Laboratories, Eindhoven

Chemical energy storage: Solid-electrolyte interfaces and interphases

- **New strategies for design of novel electrodes**
  - **Tailored architectures**
  - **Self-repairing**
- **New electrolytes: Stability at > 4 V**
- **Tailored solid-electrolyte interphase (SEI): Design of electrodes and electrolytes as a system**
- **Multi-dimensional, in situ characterization tools**
- **Computational models**

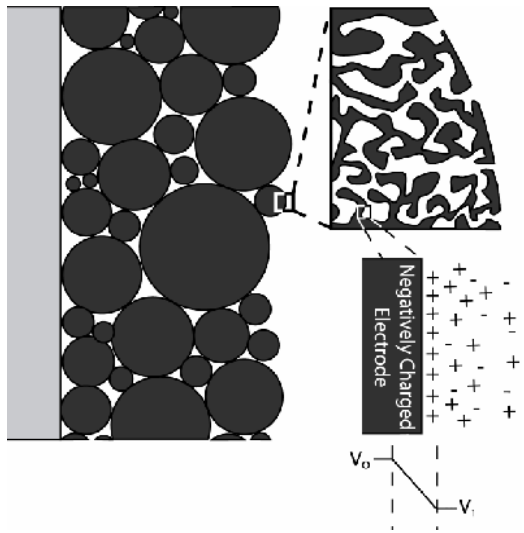


SEI stability and growth during continuous lithium uptake and removal for lithium storage metal anode

Capacitive energy storage

Materials by Design

- Materials designed with tailored pore sizes and architectures
- Multifunctional materials for charge storage using multiple mechanisms
  - Functionalized pores for higher charge density
- Computational tools optimized for capacitive storage



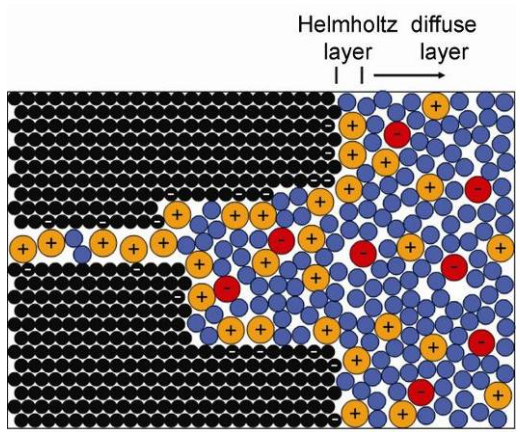
Heterogeneity of particle size, pore size, and pore structure of electrode limits performance

Electrolyte interactions

- Improved understanding of bulk phase electrolytes
  - Electrolyte/electrode interactions
- Electrodes designed to enhance pseudocapacitance
  - In situ characterization

Ion solvation may change in pores of different sizes during EDL charging

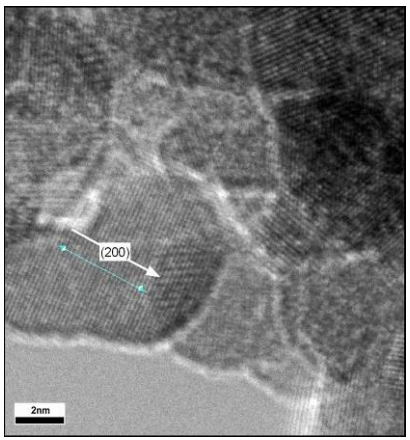
(electrode; solvent; cation; anion)



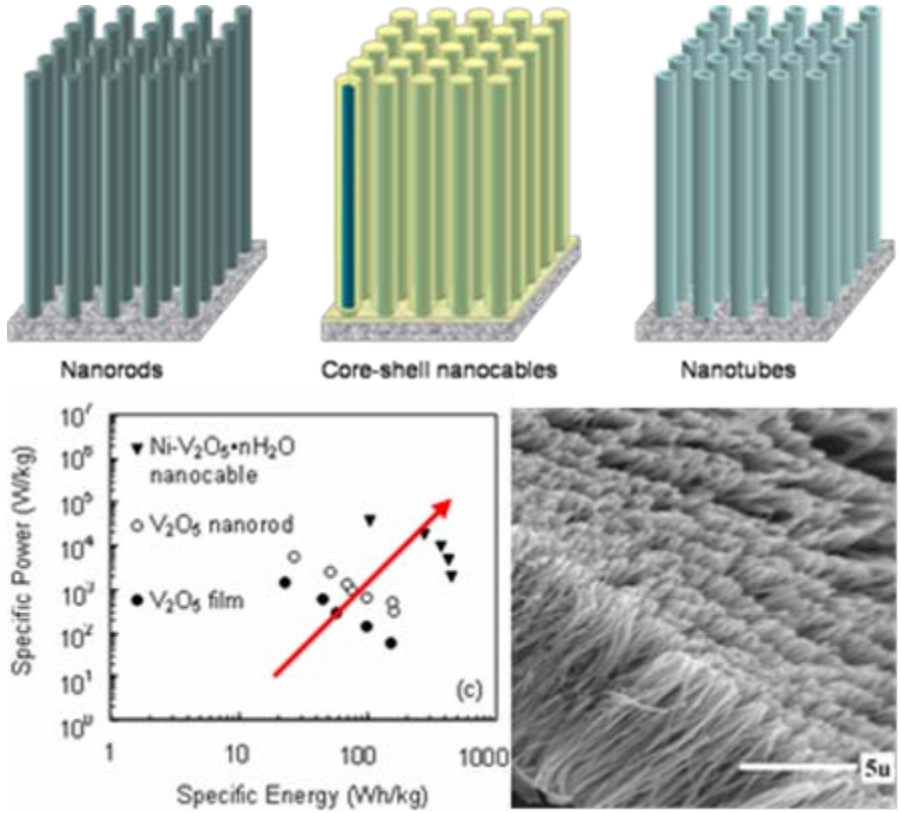
Multifunctional materials for pseudocapacitors

Objective: **Simultaneously maximize both energy density and power density, and enhance lifetime**

- **Understand fundamental charge-storage mechanisms**
- **Produce new materials with multifunctional architecture**
- **Rationally design materials and structures**



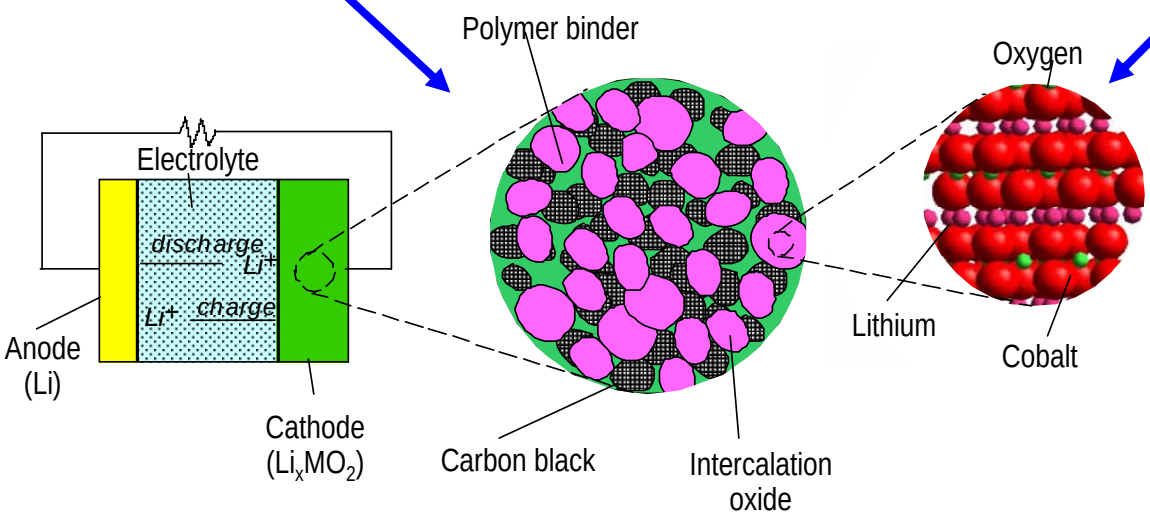
Vanadium nitride nanocrystals



Rational materials design through theory and modeling

Objective: Combined mechanical, electrical, and transport modeling of electrode

Objective: Fully predictive performance and stability modeling of active component



How to get there

- Predictive kinetics of phase changes
- Electrochemistry at the nanoscale
- Charge transport in mixed conductors
- Computational materials design
- Transport and evolution in electrode microstructures
- Structure and role of reaction interfaces

Enables:

- Modeling of performance, lifetime, and safety
- Accelerated innovation in new materials and new designs for higher energy and power at lower cost

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Work now under way supports new and expanded studies

- **Nanoscale materials and chemical sciences**
- **Diffusion and transport in fluids and ionic media**
- **Liquid / solid / gas interfaces**
- **Multiple electron redox systems**
- **Intercalation in electrode materials**

Key research questions

- **Can we develop a fundamental understanding of electronic and ionic transport in solutions and electrodes**
- **Understanding the physical and chemical processes at the electric double layer and at the electrolyte/electrode surface**
- **How to control nanostructures in multi-component, electrode/electrolyte systems**
- **How to model battery and capacitive systems across length and time scales**

Expected progress

- **One year**
  - **Prototype models of simple capacitive and battery systems**
  - **Experiments with model systems demonstrate understanding and techniques to address diffusion, EDL, interface, and solvation phenomena**
- **Three years**
  - **Competent models yield results that guide experimental directions**
  - **Experiments demonstrate promising approaches to achieve significant improvements**
- **Five years**
  - **Predictive capability for new systems**
  - **Credible approaches to transformational improvements**
- **This will require a sustained "use-inspired" basic research investment of $20-30M/year**

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