Chemical Storage Science:
Leaders: Steve Visco and Stan Whittingham

Systems	The Interface/Anode/Electrolye	The Cathode
Glenn Amatucci	**Martin Winter** (Austria**)**	**Michael Thackeray**
Khalil Amine	Austen Angell	Debra Rolison (w)
Yet-Ming Chiang	Richard Jow	Atsuo Yamada (Japan)
	Linda Nazar (Canada)	

Rational Synthesis of Materials	Characterization and Nanomaterials
Gerbrand Ceder	**Clare Grey**
Ann Marie Sastry (w)	Heike Gabrisch
Venkat Srinivasan	Robert Kostecki (w)
	Rosa Palacin (Spain)

Bold = leader; w = writer

Chemical Storage Science:
current status

Chemical Storage Science: current status

- NiMH to be replaced by Li-ion in HEVs?
- HEVs will continue to penetrate automotive markets
- If PHEV, and grid backup become commercial reality, the volume and revenue associated with battery technology will be staggering
- U.S. and Europe far behind (absent) Japan, Korea, and China in the commercialization advanced batteries.
- There is a pressing national and global need for investments in energy storage technology.
- Battery development is becoming increasingly sophisticated and as such will be driven by fundamental advances.
- Long incubation period for translation of fundamental advances to commercial reality highlights the need for immediate action.

High Performance Electric Transportation

Chemical Storage Science: technology challenges

- Increasing the energy and power density of secondary batteries without comprising safety or calendar life.
- Extremes of temperature (poor performance or premature failure).
- Cost
- Current HEVs utilize Ni/MH systems which have cost, energy content, and life limitations that prevent broad acceptance.
- Existing battery technologies do not satisfy the requirements for PHEV, or EV applications: breakthroughs are needed
- For grid backup current battery systems are life-limited and still too costly - breakthroughs are needed.

Chemical Storage Science:
basic-science challenges, opportunities, and needs

- Identification of potential "breakthrough" chemistries through fundamental science: provide guidance and accelerate the process.
- The progression to higher energy and power density batteries pushes materials to the edge of stability (energy storage must be safe, long-lasting and inexpensive).
- Thermodynamic and kinetic data to guide system design & elucidate rapid self-disassembly (flamethrower laptops).
- There is a pressing need for in-situ tools and approaches to look at the structure and stability of interfaces and dynamic processes under realistic conditions
- Explore and understand fundamental life-limiting phenomena in multi-component battery materials and systems.
- A theoretical description of the SEI (solid electrolyte interphase).

Chemical Storage Science:
basic-science challenges, opportunities, and needs

- **The use of computational tools to predict properties and guide rational design**
- **Exploit advances in characterization tools to expose underlying phenomena that limit life and performance and integrate this information with computational modeling work for validation and predictive fidelity.**
- **Explore and elucidate the role of nanomaterials in chemical energy storage**
- **International collaboration**
- **Feedback loop from basic science through engineering and development to validate models**

Chemical Storage Science:
Novel System Design Towards Performance and Efficiency

Scientific challenges

New fundamental understanding of the interplay of materials and charge transport for electrochemical energy storage systems enabling:
• Ultra high energy and power density
• Robust, long life and safe
• Low lifetime cost

Summary of research directions

• Multifunctional components and materials
• Higher voltage energy density multielectron redox electrodes
• New electrode and cell designs and processes inspired by nature
•Novel electrochemical couples for Li, non-Li, and flow batteries

Potential scientific impact

• New understanding of mixed conductivity and transport in macro and nanocomposite electrodes and polymers

• New understanding of the physical integration of structure and high degrees of charge transfer

• Novel multifunctional design motifs which may impact other energy technologies (PV, electrochromics,etc.)

Potential impact on EES

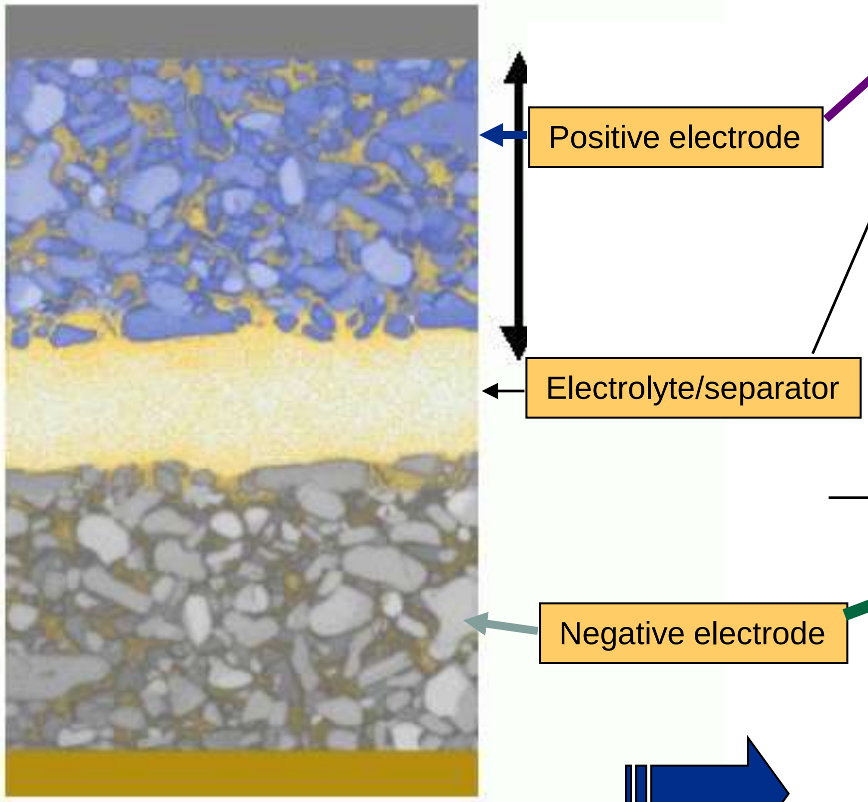
Elimination of inactive non-redox components
• improved energy density and lower cost

Multifunctional Separators and Binders
• polymer with shuttle capability, getters and dendrite control
• improved safety and efficiency

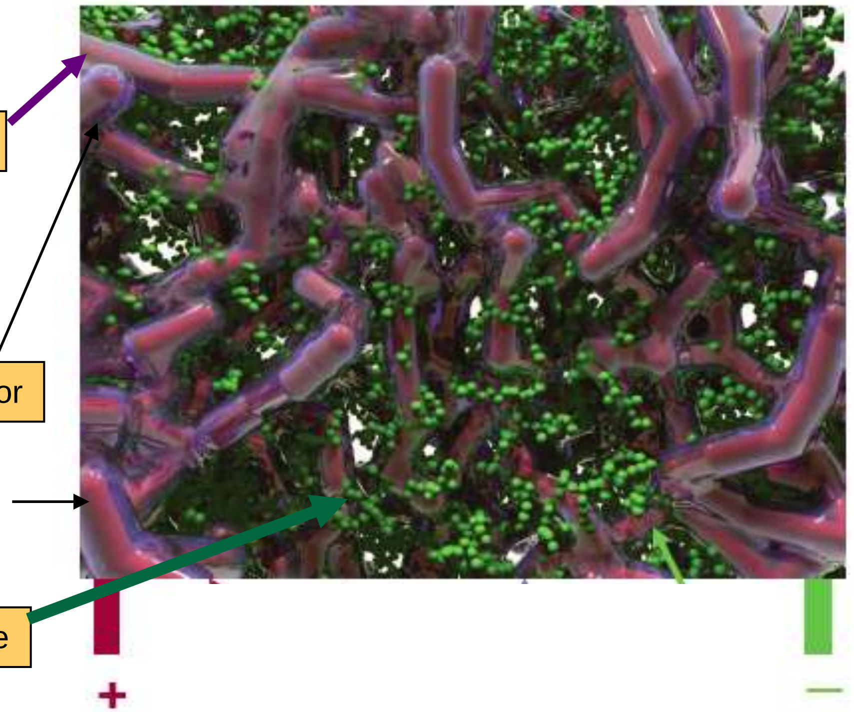
Extreme energy and power density
•Enabling new application, functionality and performance of power systems for transportation and grid

3-D and Self Assembled batteries
• lower cost and higher efficiency

Chemical Storage Science:
technology challenges



Present day Electrochemical Cell Structure



3-D Battery Self Assembled Electrochemical Cell Structures Containing Multifunctional Components.

Chemical Storage Science:

PRD: New Materials, Chemistries and Strategies

Scientific challenges

- Electrode capacity limitations (energy)
- Design stable electrode-electrolyte interfaces
- New materials/electrochemical couples required for 'beakthrough' improvements through innovative synthesis procedures
- Paradigm shift away from conventional solid state

Summary of research direction

- Create/tailor high potential materials (4.2-5.5 V vs. Li^0) with >1 e^- transfer per redox center
- Design nanomaterials to increase capacity and power and fabricate multifunctional surfaces
- In-situ measurements of dynamic processes
- Model structure, ion transport, electrode design to maximize performance
- Explore recyclable chemistries, e.g., composites, organics, liquids, metal-air (Li/O_2)

Potential scientific impact

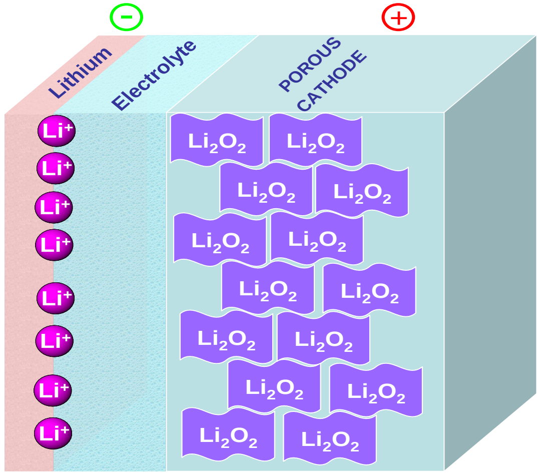
- Understand electrochemical phenomena at the nano-scale
- New synthetic strategies and processes for particle, morphological and functional control
- New structural configurations for superior hydrogen storage, catalysis, supercapacitors

Potential impact on EES

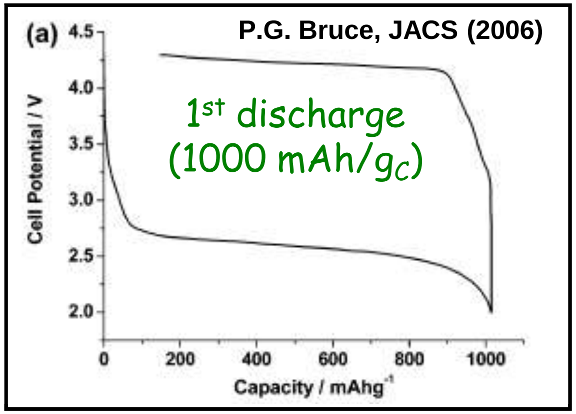
- Improve energy, power, safety, efficiency, life, operating temperature, cost
- Enable related energy technologies
- Timescale for success: 10 years or more

Chemical Storage Science:
PRD: New Materials, Chemistries and Strategies

Li/O_2 cells: A step towards the holy grail?



Proof of concept

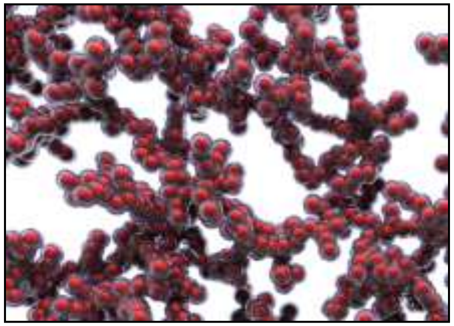


Future direction

$$2\,Li + O_2 \underset{}{\overset{MnO_2}{\rightleftharpoons}} Li_2O_2$$

(1169 mAh/g)

- Design nanomaterials to increase capacity and power and design multi-functional surfaces



Design of porous catalyzed 3-D nanoarchitecture as air cathode

- New electrochemical couples required for 'breakthrough' improvements
- Paradigm shift away from conventional solid state

Chemical Storage Science:
Rational Design of Interfaces and Interphases

Scientific challenges

Understand interface/interphase dependence on electrode materials, electrolyte components & additives (intra-cell and intra-electrode)

Separate the impact of the interface/interphase from the cell level behavior

Elucidate the role of the electrode interface in governing charge-transfer to solid-state and liquid-state electrolytes

In-situ probes of interface behavior

Potential scientific impact

New discoveries will lead to advances in other field involving charge-transfer interfaces

New dynamic in-situ probes will impact other interface-dependent fields (fuel cells, electrocatalysis. biological membranes)

Summary of research direction

Strategies for electrode-electrolyte synergy for novel non-carbon anodes and next-gen cathodes

Design of new anodes, solvents, salts and additives for SEI stabilization and wide temperature/ large potential window operations

Understand electrode/ electrolyte (SEI) and intra-electrode interfaces (active↔binder↔conductive add.)

Develop characterization tools and approaches to probe the interface under dynamic conditions

Potential impact on EES

Tailor-designed interfaces for future energy storage systems

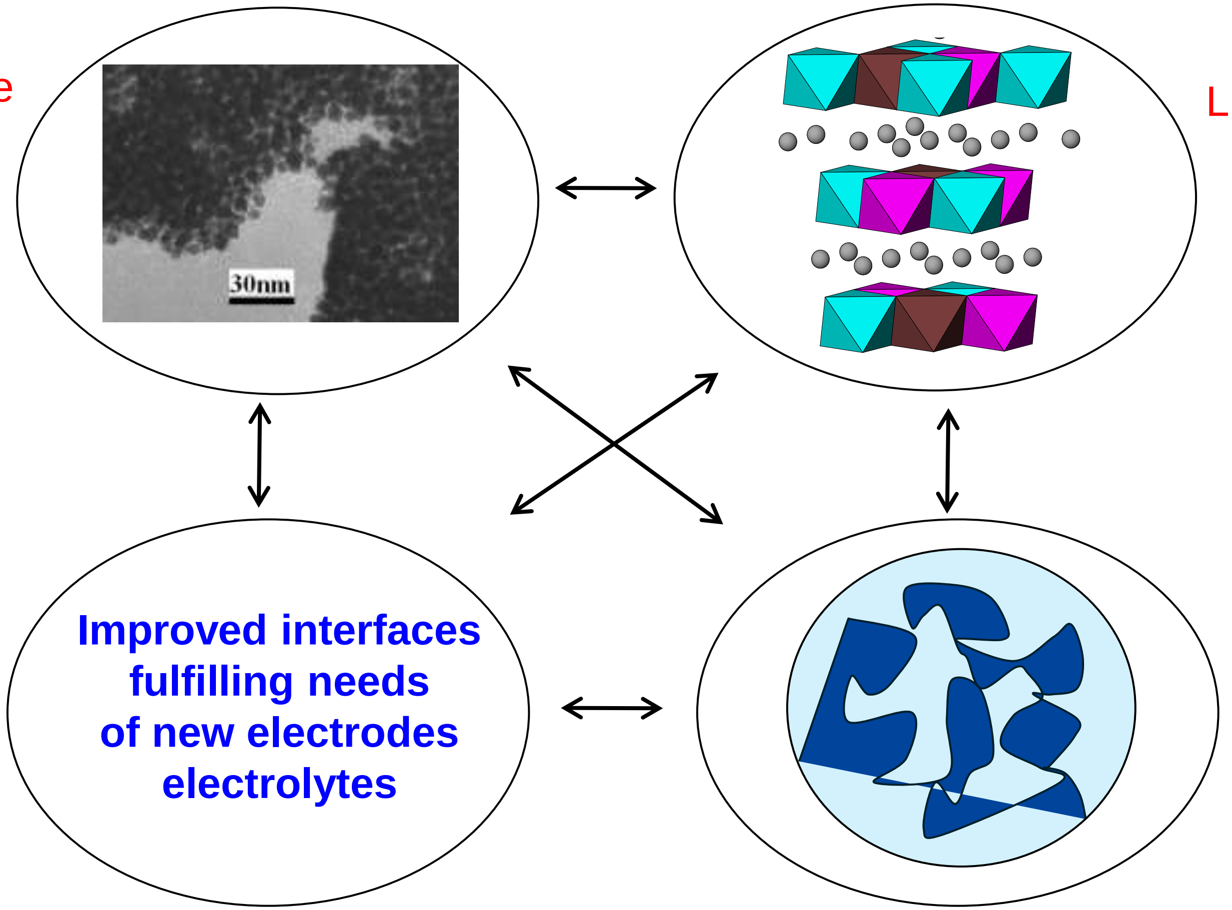
Longer life and safer energy storage systems that provide higher energy density

Chemical Storage Science:
Synergetic Electrode-Electrolyte Research

1991
- 2007

new composite alloy anodes
↑
graphite

$Li[Co_{1/3}Mn_{1/3}Ni_{1/3}]O_2$
↑
$LiCoO_2$

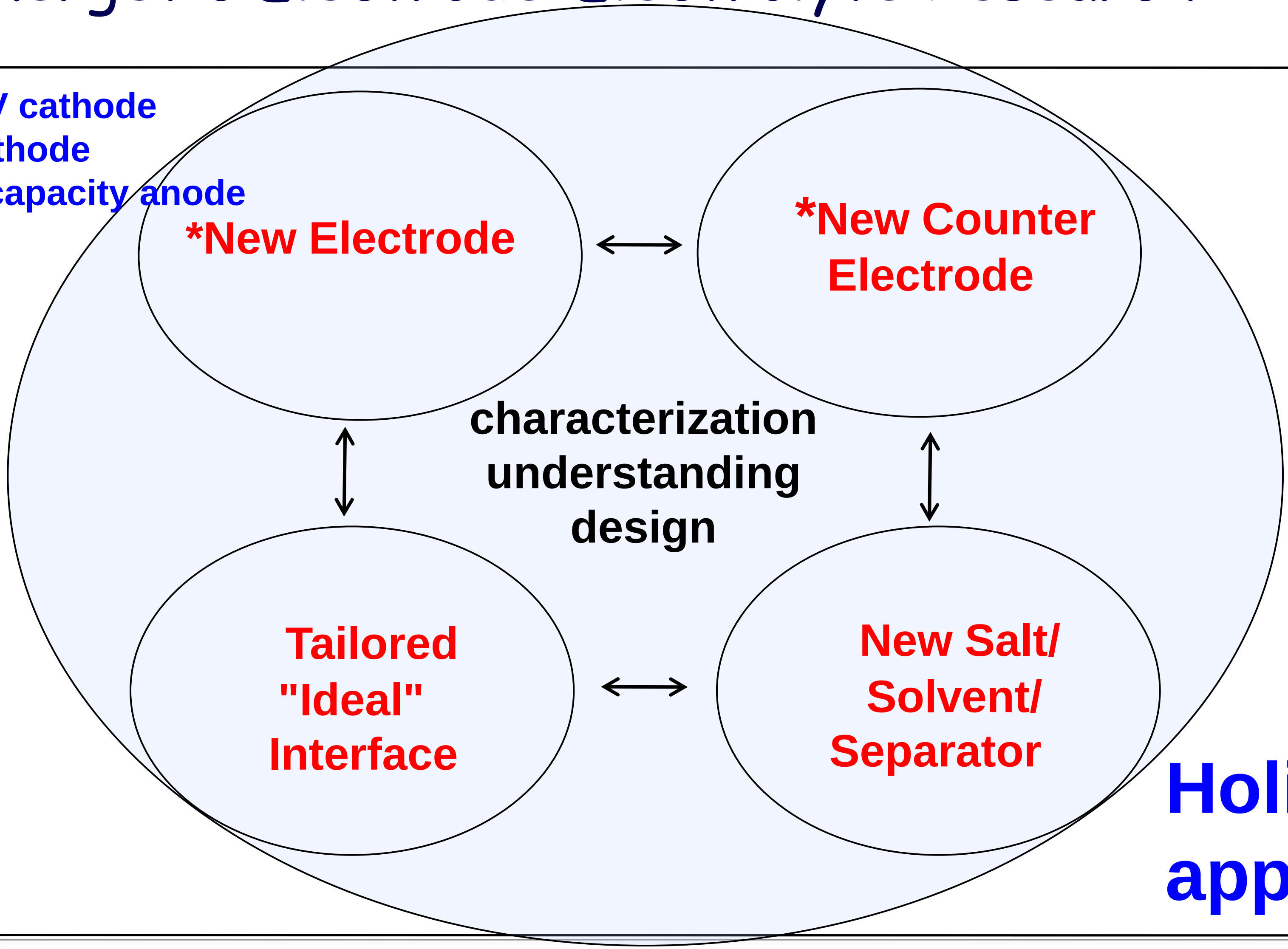


Oxidative resistant polymeric gel Separator + higher V electrolyte
↑
microporous polypropylene + EC/DMC

Chemical Storage Science:
Synergetic Electrode-Electrolyte Research

1991 - 2007

- high V cathode
- air cathode
- high capacity anode
- Etc.

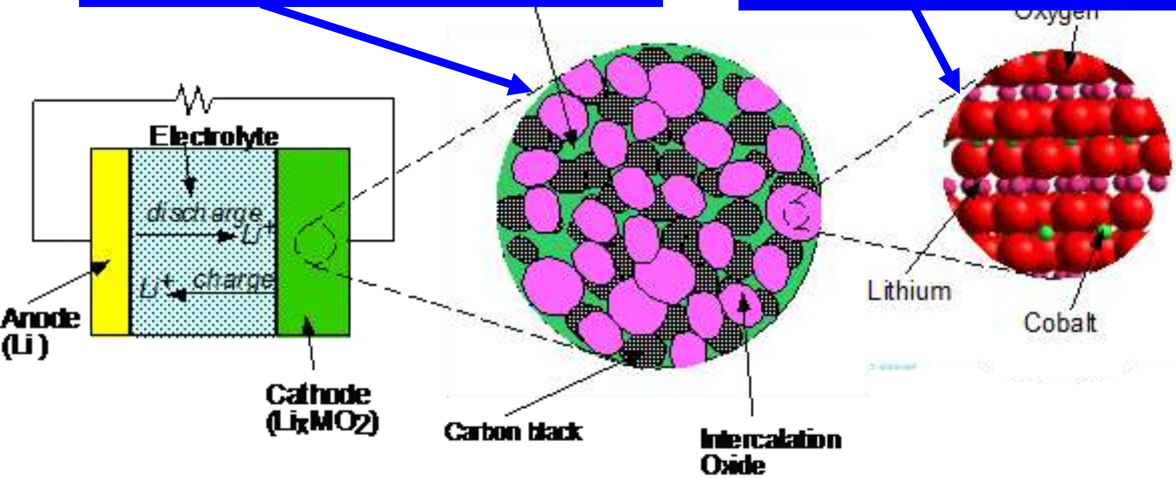


Holistic approach

Chemical Storage Science:
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 nano-scale
- Charge transport in mixed conductors
- Computational materials design
- Transport and evolution in electrode microstructures
- Structure and role of reaction interfaces (SEI)

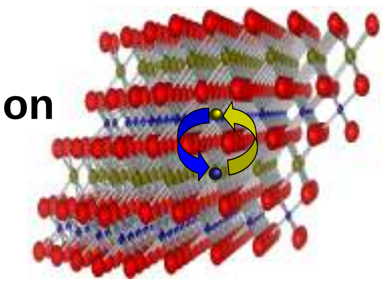
Enables:
Modeling of performance, lifetime and safety
Accelerated innovation in new materials and new designs for higher energy and power at lower cost

Chemical Storage Science:
Rational materials design through theory and modeling

Scientific challenges

Development of knowledge and computational tools to predict properties, performance, evolution and lifetime of materials for chemical energy storage

vision: computationally driven materials design and analysis



Summary of research direction

- Predictive Kinetics of phase changes
- Transport and evolution in electrode microstructures

Structure and role of reaction interfaces (SEI)

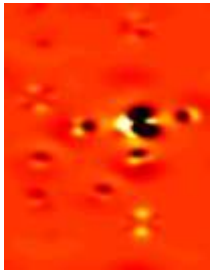
- Electrochemistry at the nano-scale
- Charge transport in mixed conductors
- Inverse and computational materials design
- Modeling of spectroscopic methods

Potential scientific impact

Insight into behavior of nanomaterials

Novel numerical techniques for integrated kinetics modeling in multi-phase systems.
Impact on other fields

Computationally driven materials design



Potential impact on EES

- Higher **energy** and **power** density storage
- Accelerated lower cost design of **novel materials** and rapid screening of new ideas
- Prediction of **lifetime and failure mechanisms**.
- Enable evolution from microscopic to molecular design and **assembly of batteries**

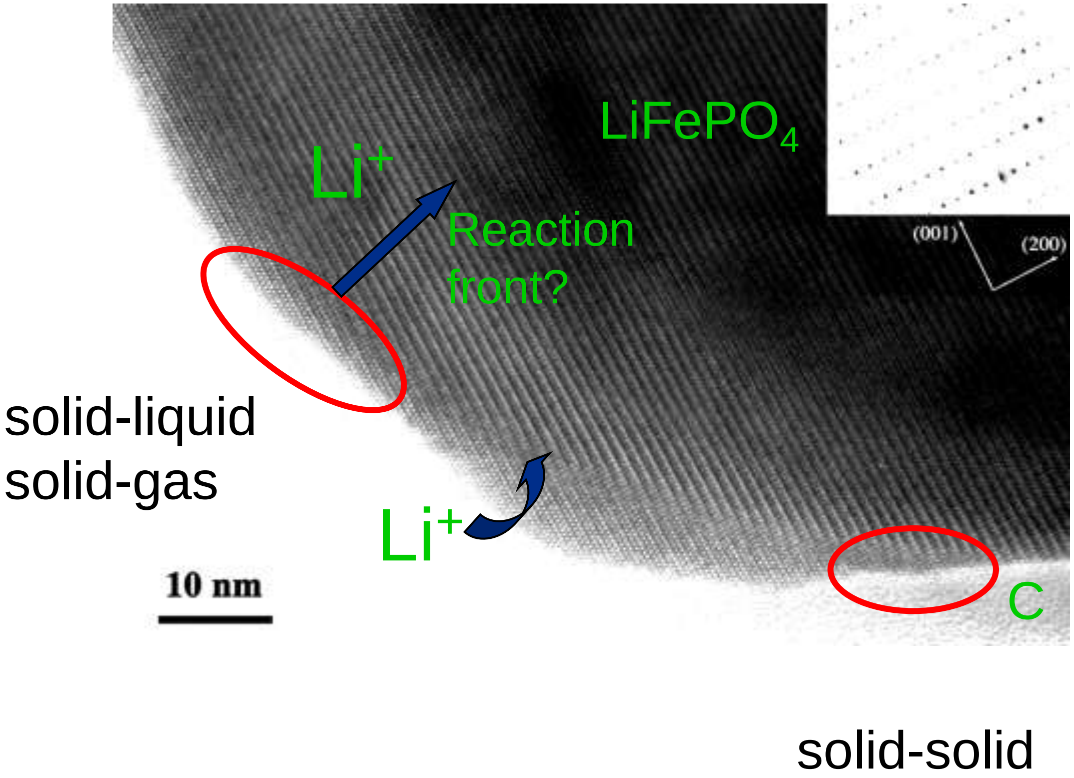
Chemical Storage Science:
Novel Characterization Approaches

Scientific challenges

Interfacial structure and processes:

- How do we characterize local processes with increased sensitivity, in real time?

- **How do we identify the important phenomena that occur over wide ranging timescales, and that contribute to battery failure?**

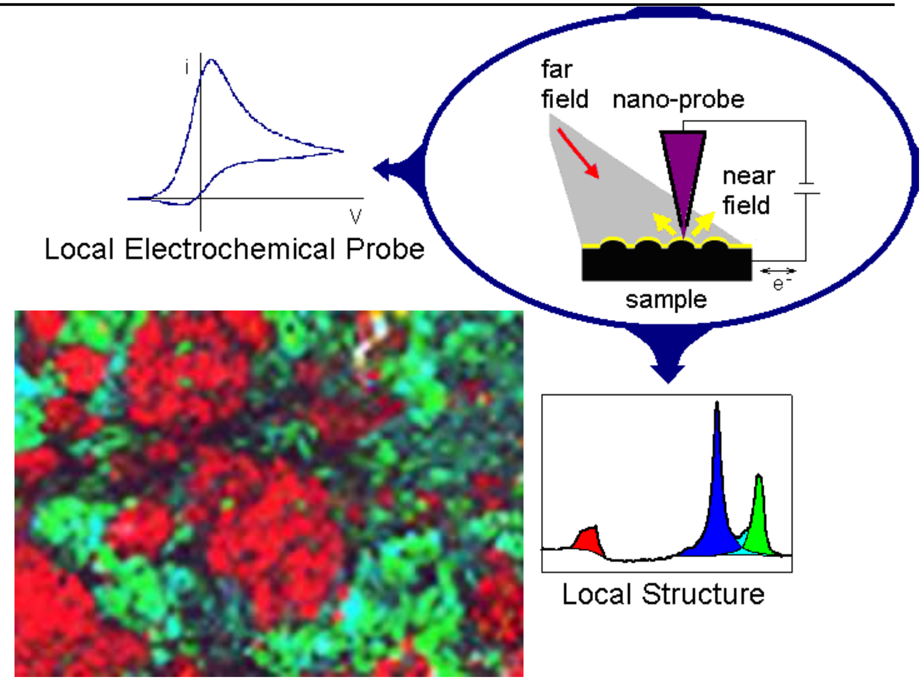


Chemical Storage Science:
Novel Characterization Approaches

imaging + spectroscopy

Summary of research directions

- Multi technique, *in situ* methods…. sensitive to structure and dynamics at interfaces
- Push timescale (fs – s) of *in situ* methods
- Examine response to electrochemical perturbations
- Couple with theory
- Design model experiments to extract different lifetime-dependent failure modes



Potential scientific impact

- Fundamental understanding of intercalation/conversion reactions
- Ability to tune and design interfacial processes
- New time- and spatially- resolved techniques to examine interfaces

Potential impact on EES

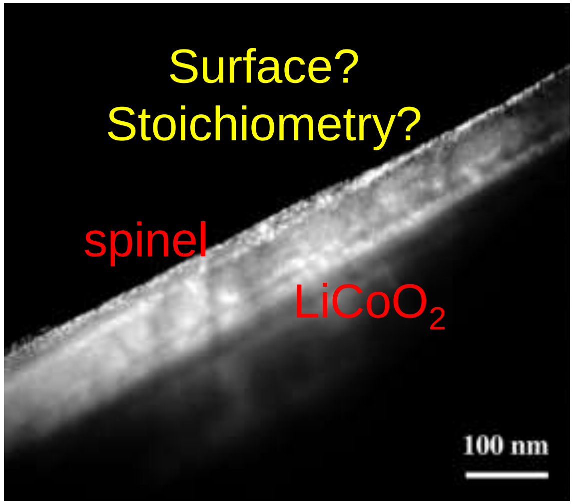
- Revolutionize the design of interfaces, surfaces, morphologies
- Rational design of high-rate materials with longer lifetimes

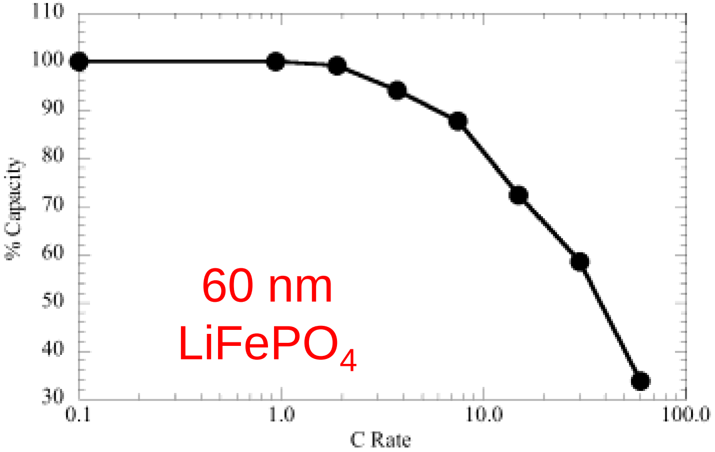
Chemical Storage Science:
What makes nano different for chemical energy storage?

Scientific challenges

Understand phenomena at the nano-to-atomic lengthscale and the consequences of utilizing nanoparticles and composites in battery systems

- Exploit rapid reaction kinetics to enable new electrochemistries?
- Pseudo-capacitive vs. storage effects?
- How do we characterize nano particles and composites?
  Structure at the 5 Å – 5 nm length scale?





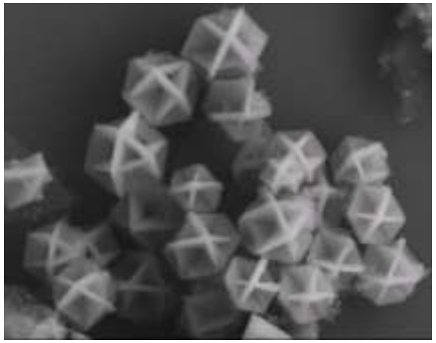
Transport?

Structural relaxation?

Electronic?

M. S. Whittingham, J. Mater. Chem., in press (data from Kim &Kim)

Chemical Storage Science:
What makes nano different for chemical energy storage?



Summary of research direction

Characterization:

- Develop local structural and interfacial probes and tools that separate surface and bulk effects.
- Combine multiple structural probes

Synthesis:

- Engineer particles, heterostructures, and composites with new morphologies, controlled sizes, engineered surface properties, to develop new properties and understand properties

Modeling:

- Push method development and application to understand structure/electronic size effects

Potential scientific impact

- Fundamental understanding of nanoscale phenomena
- Extensions to interfacial processes in related fields, e.g., catalysis, fuel cells, PV cells etc.

Potential impact on EES

- *New* electrochemical processes and storage mechanisms
- Higher rate batteries