Energy Storage Beyond Li/ion Batteries

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cient electrical energy storage

lay's electrical energy storage (EES) technologies fall far
ort of requirements for efficient use of electrical energy

volutionary 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

s will require transformational
ances in the underpinning of materials
l chemical sciences

- Significant advances in the fundamental understanding of nanosc
phenomena
- Predictive modeling of complex, multi-component systems over multiple length and time scales

tablishing a scientific foundation technology breakthroughs

ory, modeling, and simulation
plement experimental efforts

nsight into novel
charge storage mechanisms

Prediction of trends

Design criteria for new materials

Guidance for experiments

Ability to address a broader range of materials
ystems and compositions

e multiscale computations
provide fundamental understanding
rocesses

Phase transitions
n electrode materials

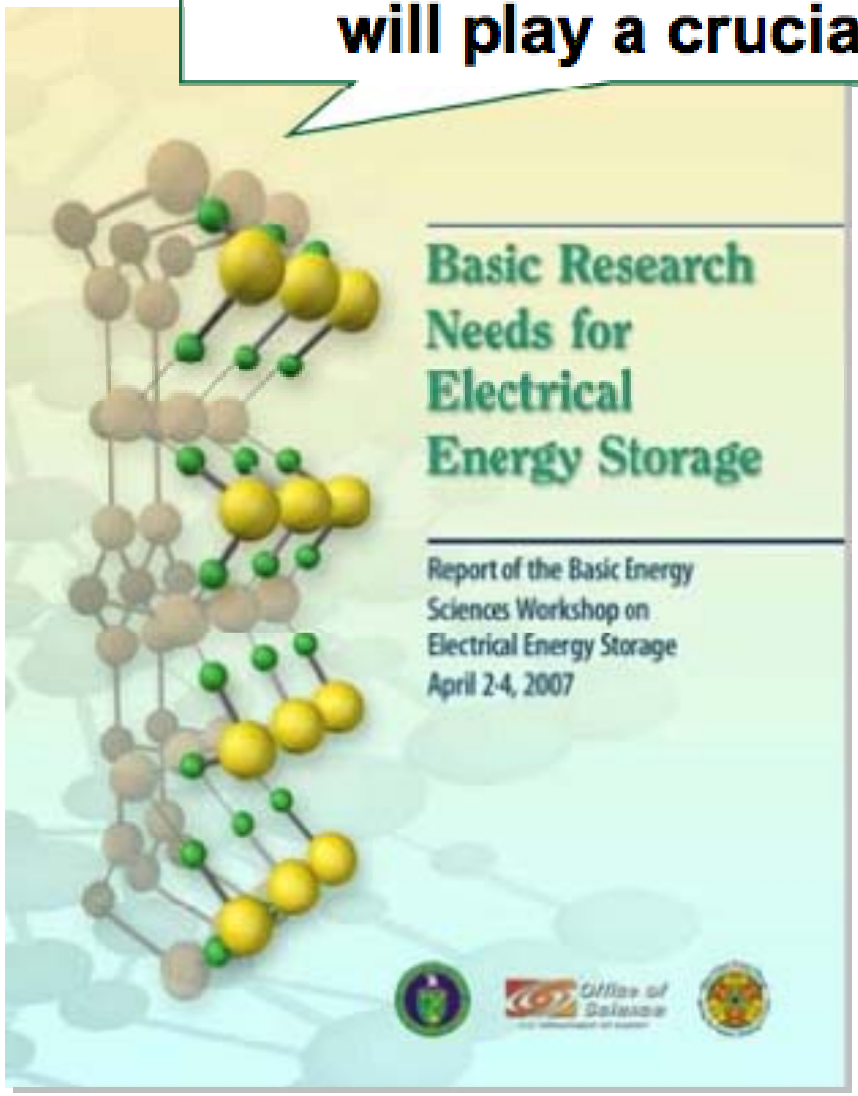
on transport in electrolytes

Charge transfer at interfaces

Electronic transport in materials

Evaluation of complex systems

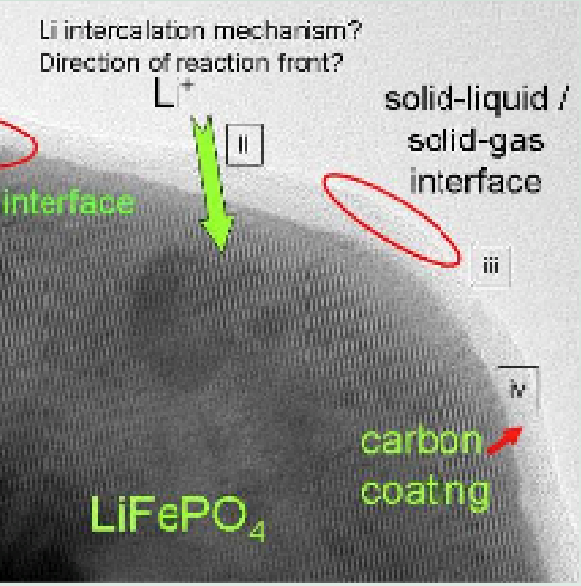
"New computational me
will play a crucial ro



http://www.er.doe.gov/bes/reports/files/EES_rpt.pdf

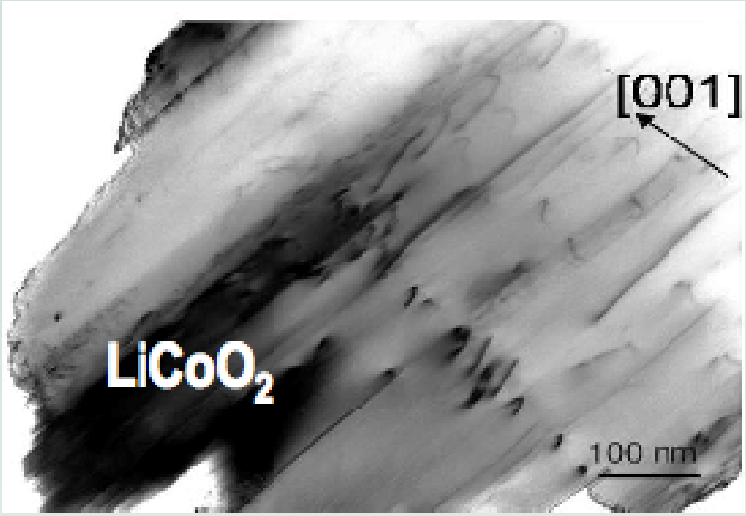
damental challenges

vledge gap: Basic understanding of the mechanisms
netics of the elementary steps involved in chemical storage



o correlate interface ure with reactivity?

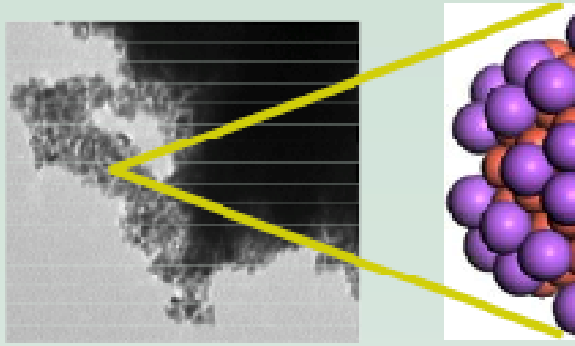
molecular-level standing of ion alation or reaction id-liquid s-solid interface



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 betw nano and bulk?

Novel ideas needed to handle nanoscal relevant to technolo (10–150 nm)

st be addressed

ase energy and power density
ut compromising safety or lifetime

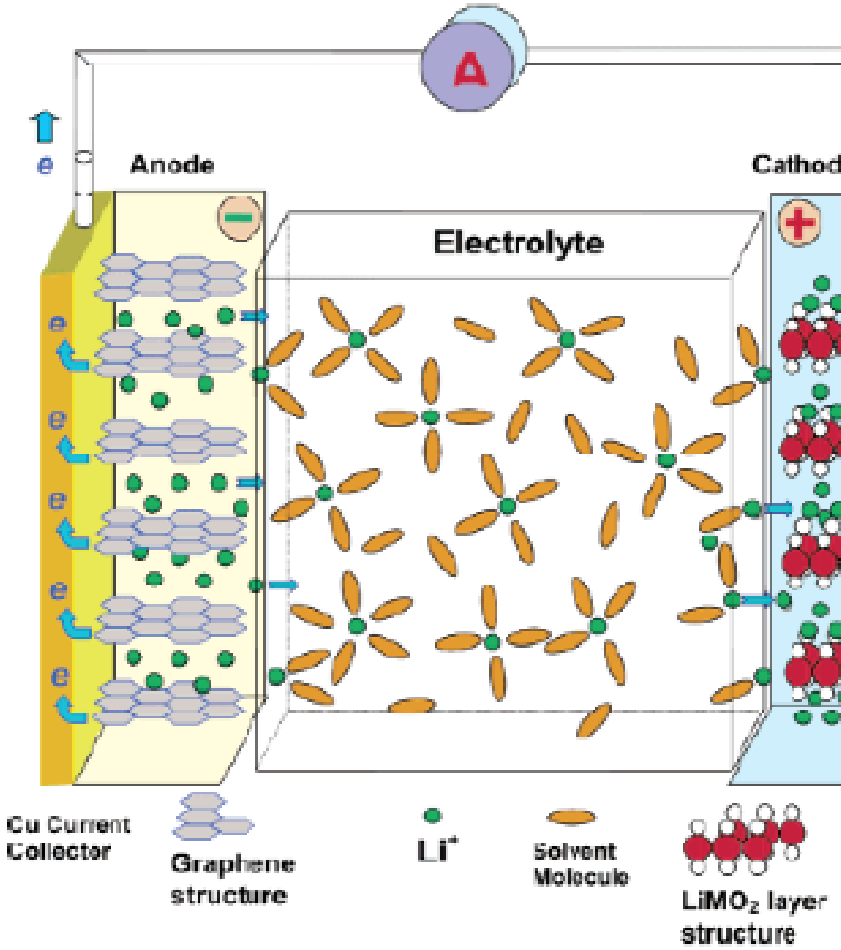
er faster charge cycle times

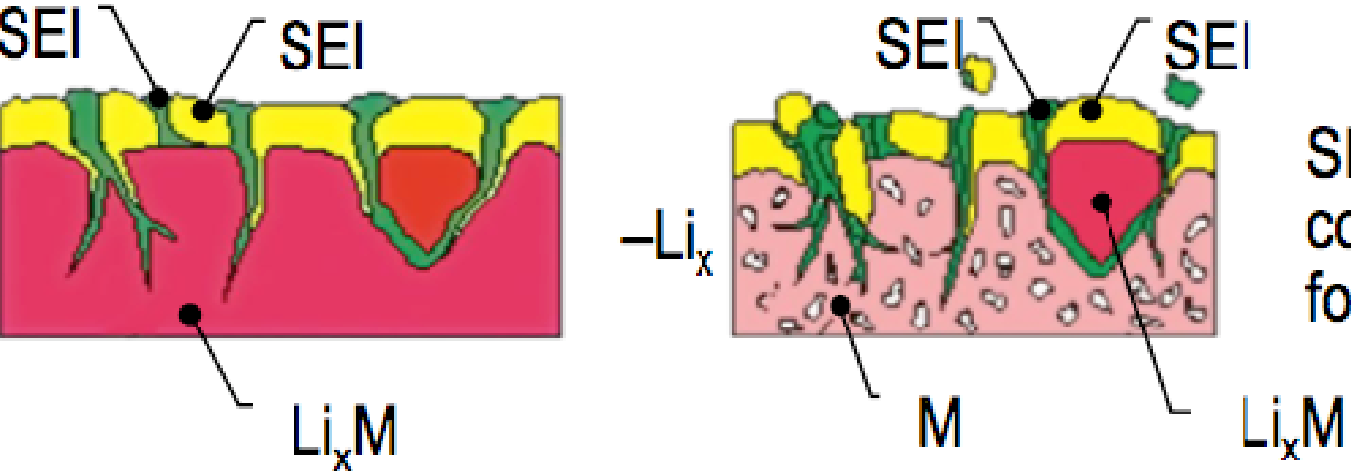
rements:

reakthroughs in materials
nd chemical processes

nderstanding of solid-electrolyte interface

ontrol of charge transfer





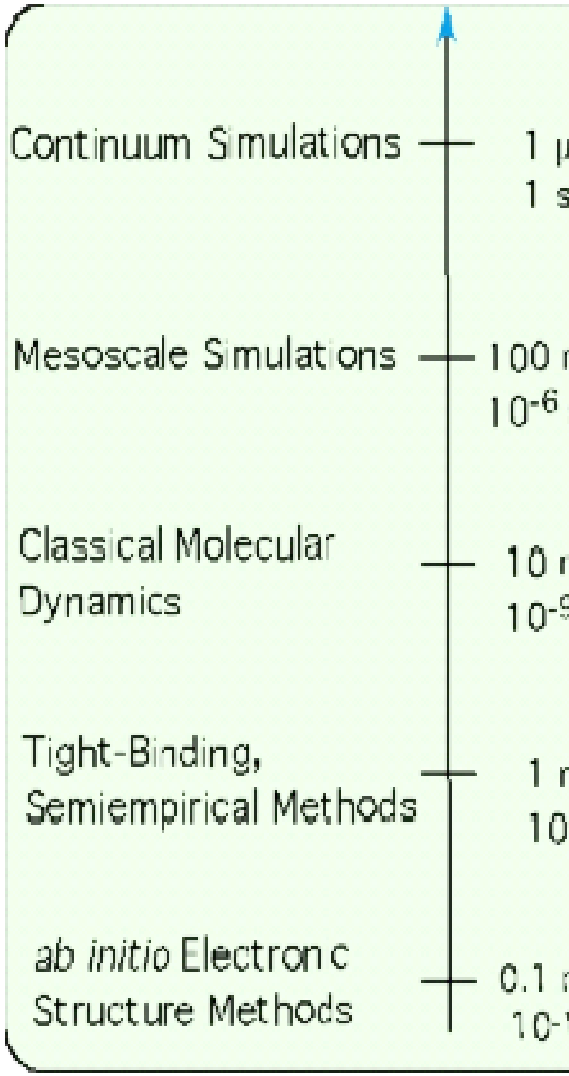
SEI stability and growth during
continuous lithium uptake and re
for lithium storage metal anode

e cross-cutting challenges for computation simulations requ aking REVOLUTIONARY breakthroughs in battery and capa research

Merging of new theoretical methodologies to xplore the complexity of physical and hemical processes occurring over the full ange of length and time scales

Multi-scale modeling for the virtual design of naterials with user defined properties

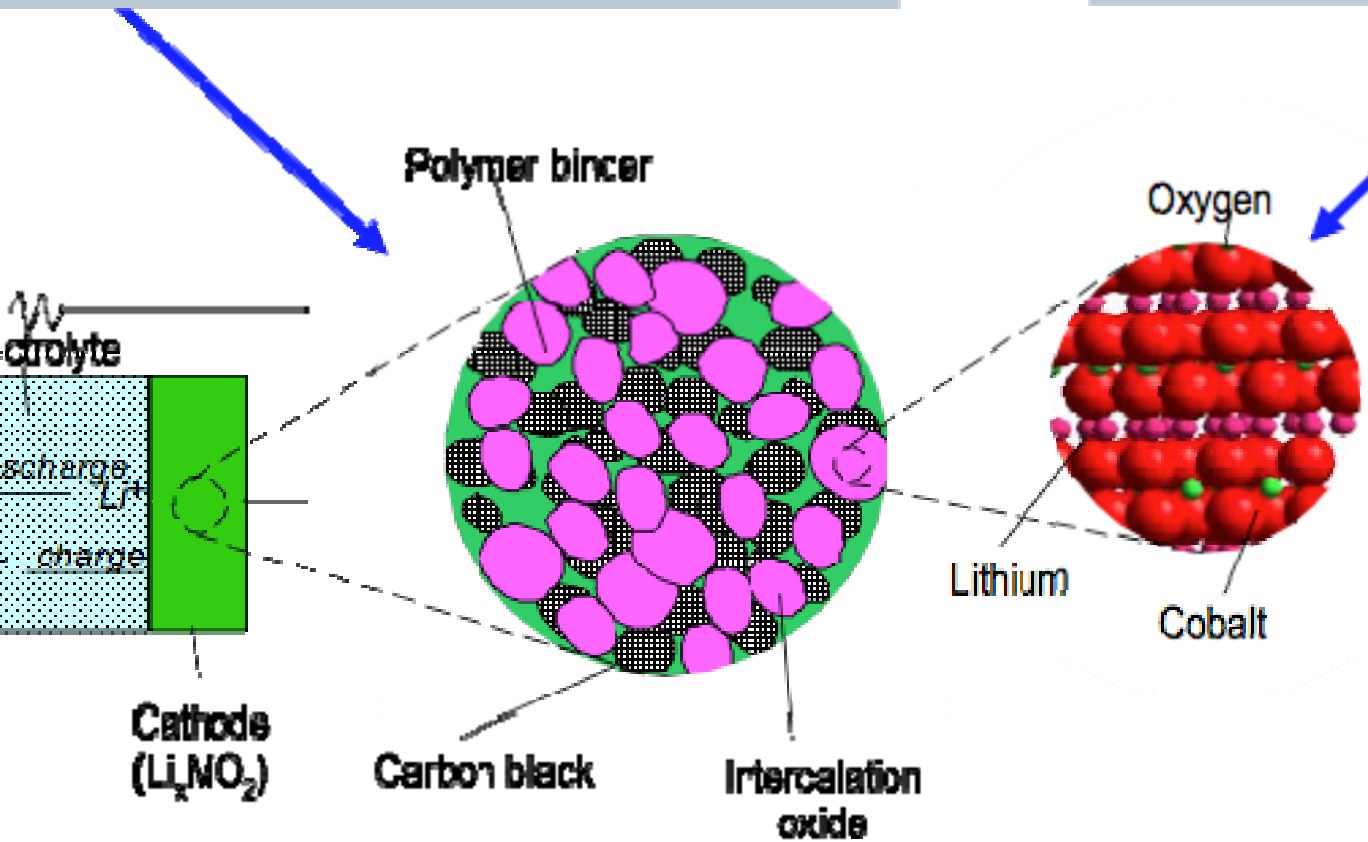
Computer simulation for prediction of ustainability, risk, and life cycle analysis



ough theory and modeling

tive: Combined mechanical, al, and transport modeling rode

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 evolutio in electrode microstruc
- Structure and role of reaction interfaces

es:

ing of performance, lifetime, and safety

erated innovation in new materials and new designs

gher energy and power at lower cost

an we develop a fundamental
nderstanding of electronic and ionic
ansport in solutions and electrodes

nderstanding the physical and chemical
rocesses at the electric double layer and a
e electrolyte/electrode surface

ow to control nanostructures in multi-
omponent, electrode/electrolyte systems

ow to model battery and capacitive system
cross length and time scales

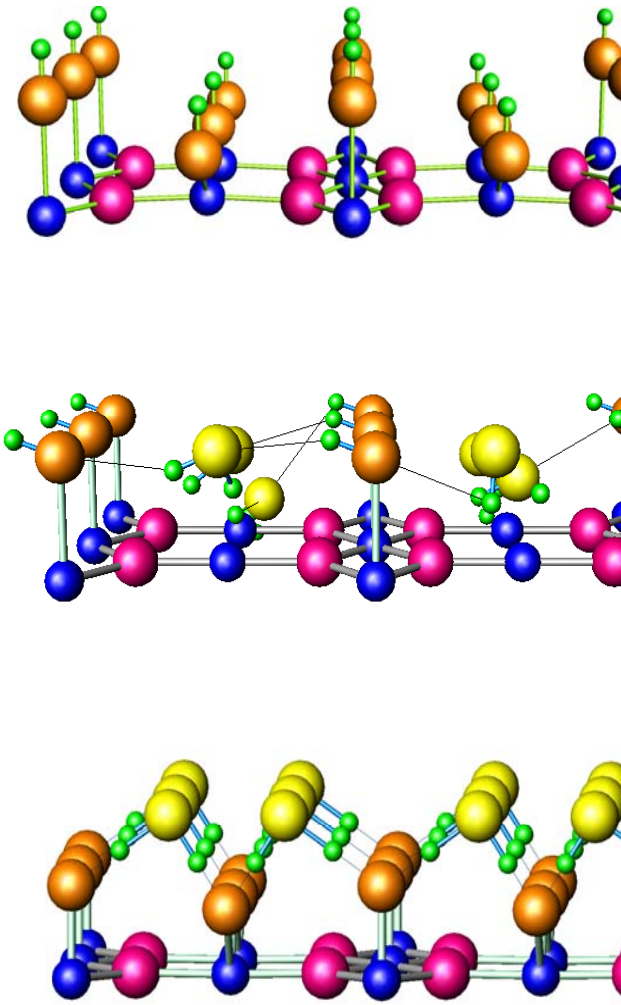
ling support required to successfully ess computer modeling challenges

ensive collaboration with characterization entists, e.g., neutrons, x-rays, electrons, and ectroscopy

lidation with experiment on model systems to sure reliability of computational simulations.

gh-performance computing

sources to train a new generation of scientists fundamental research on electrical energy rage systems



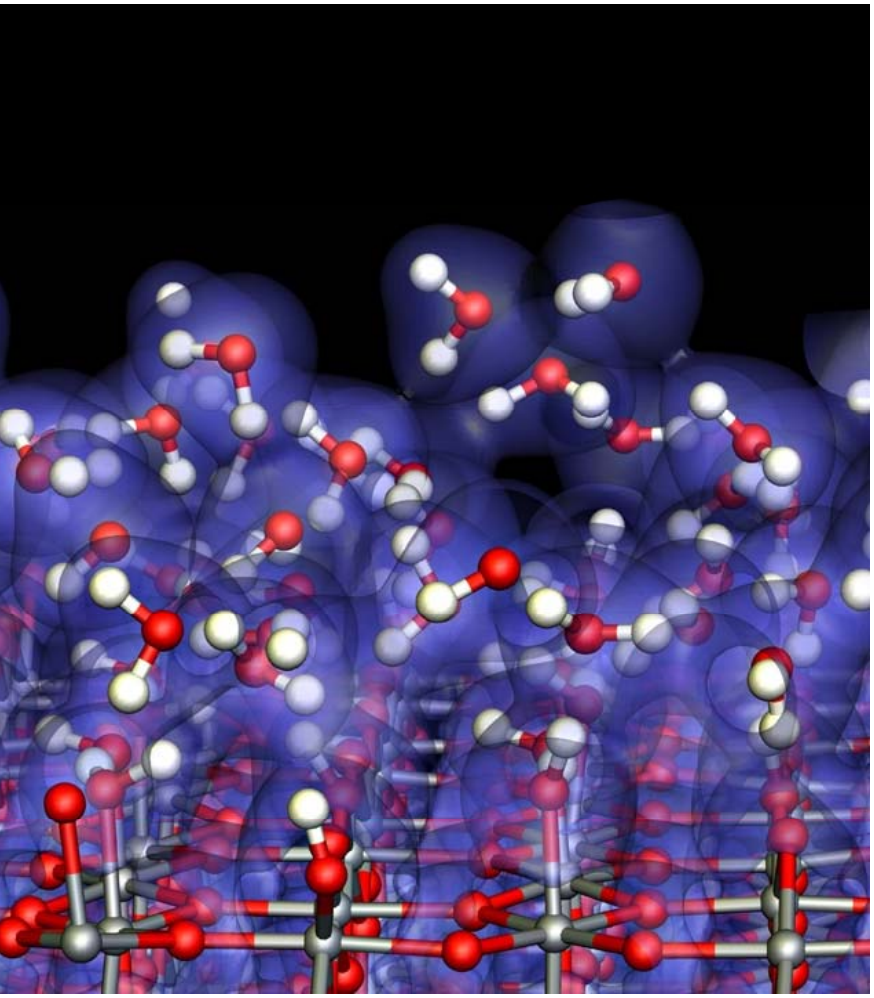
Formation and destruc of water monolayer on surface from theory an experiment

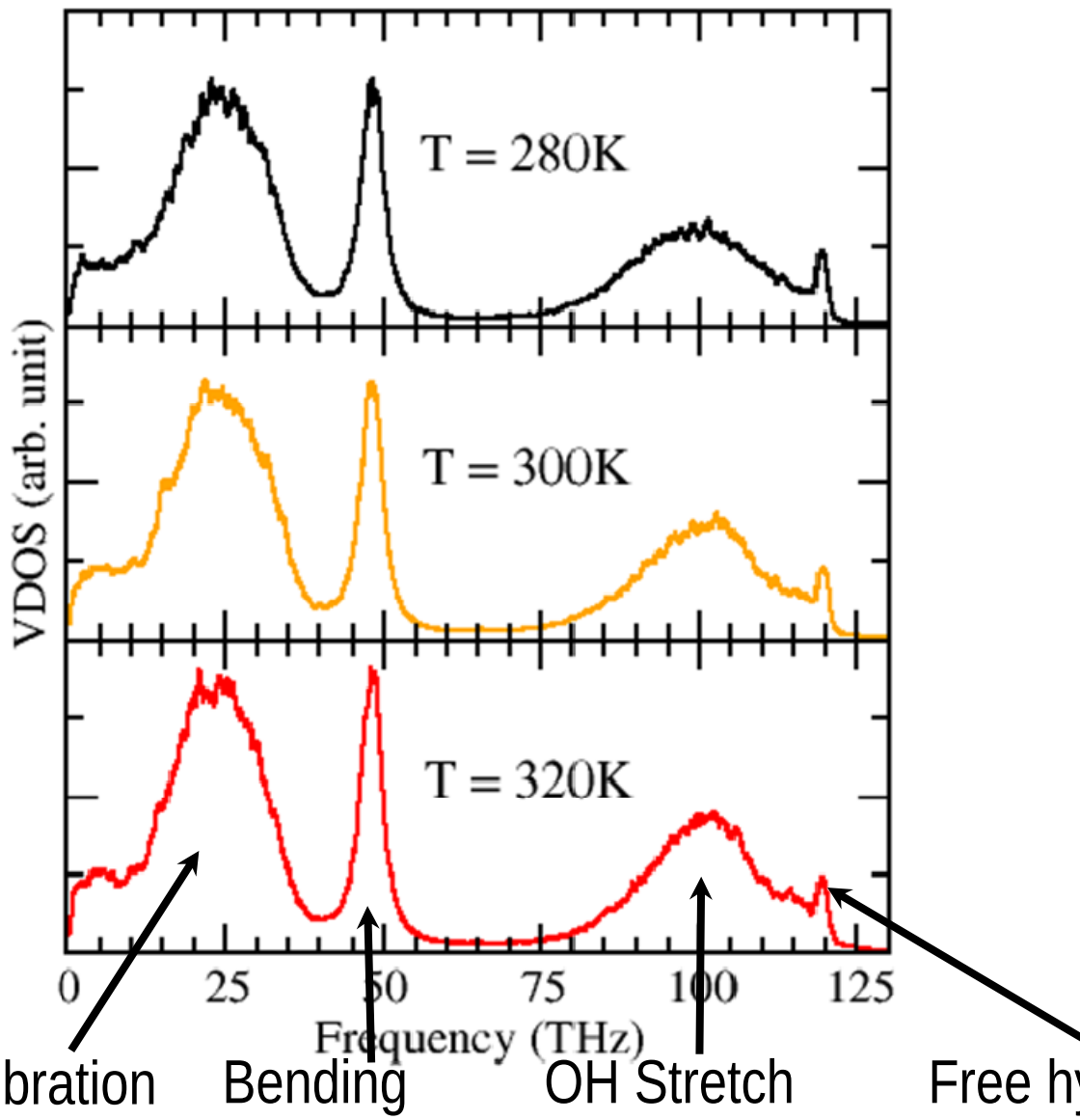
of water at oxide surfaces

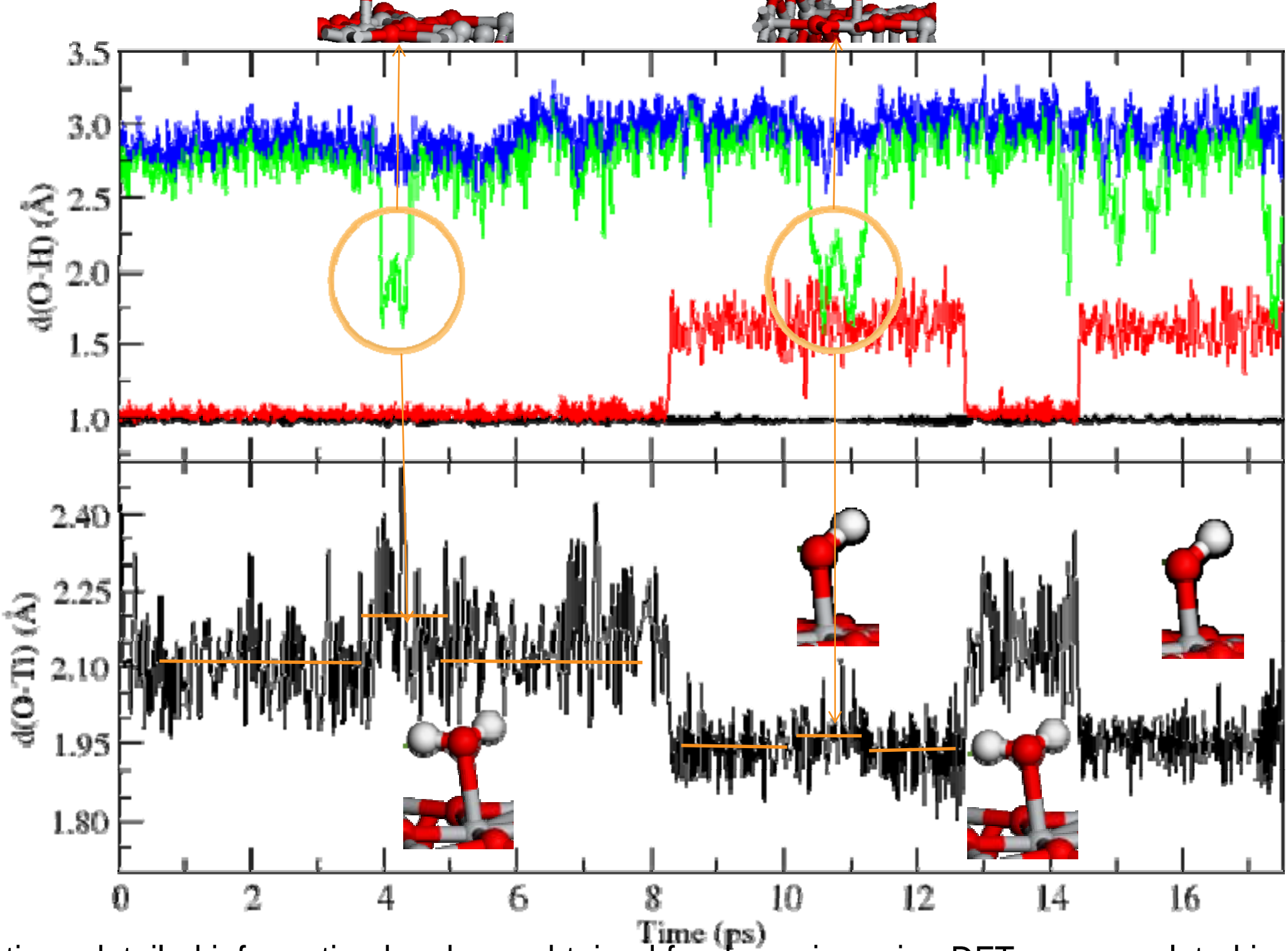
Movie

llustrates time and lengthscale challenges

long-time DFT based molecular dynamics calculations provide detailed information on the s
protonation/dissociation level) of water on (110) rutile. Simulations are validated using x-ray
tering data. Calculations are being extended to other oxide/mineral surfaces.







st time, detailed information has been obtained for dynamics using DFT, e.g. correlated jump
ond lengths with changed coordination. Simulation averaged adsorbed Ti-O bond length ad

Basic Science Challenges, Opportunities, and N

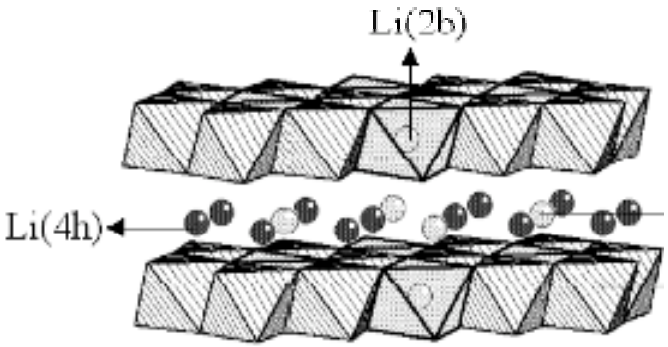
odeling of kinetics and dynamics of phase nsformations in electrode materials and ectrolytes

gh-throughput virtual screening of aterials and devices for batteries and pacitors

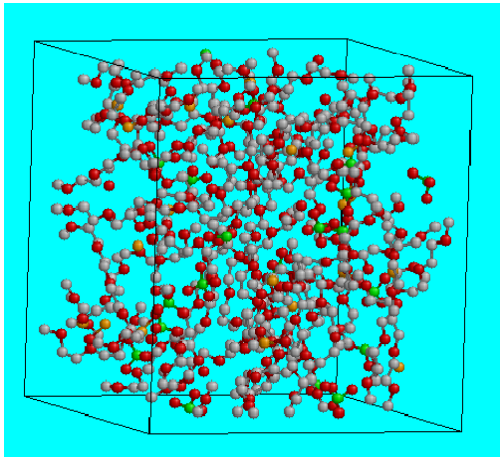
esign and construction of materials with sired electrical storage properties using ultiscale modeling

nderstanding charge transfer and transport electrical storage materials

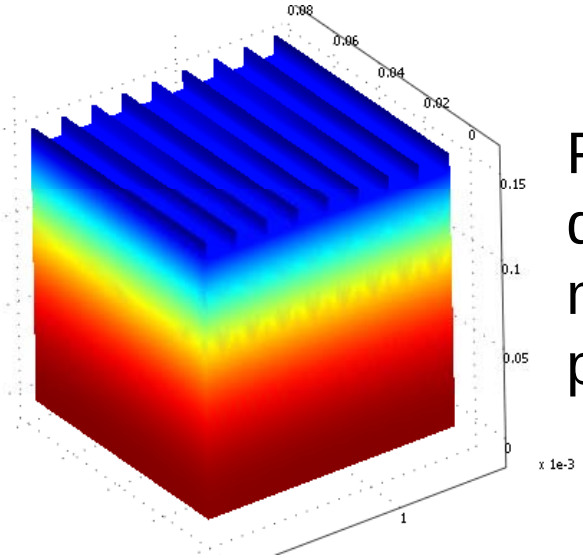
egrating modeling of nanoscale and acroscale effects



Predicte position



MD simu $LiClO_4$/P polymer electroly



Predicte distributi multi-ele pouch c

ving Questions

spatio-temporal change of charge distribution at
ondary particle-level on full-cell performance
e of 3D geometries on the energy and power

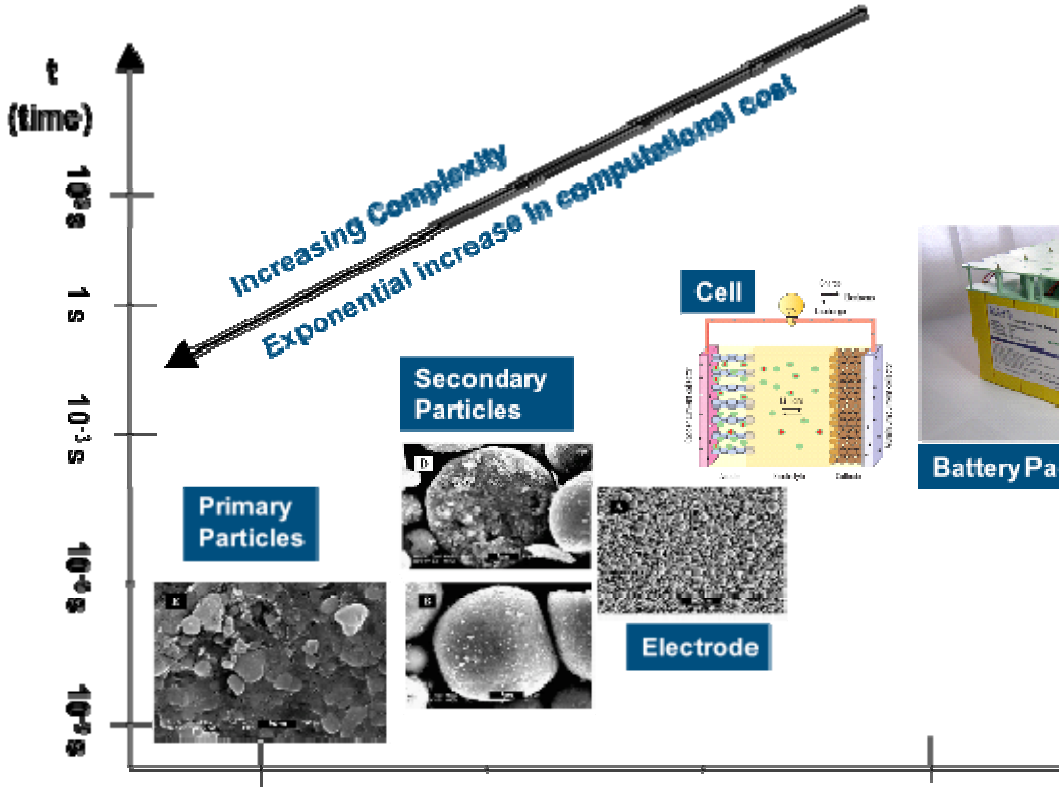
D interactions between charge transport, local
try, mechanical properties, cyclability,
nance and safety

A Challenging Problem

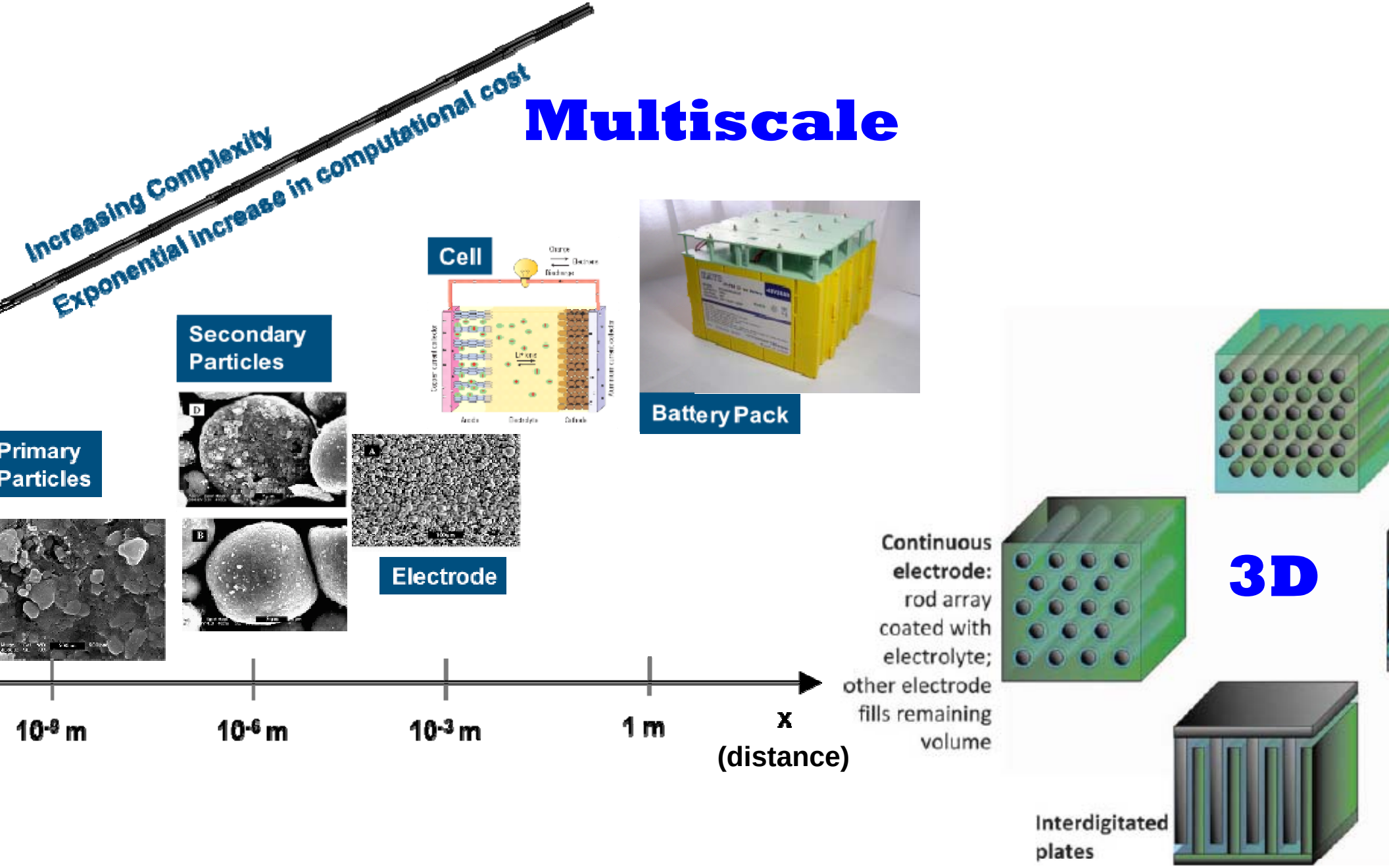
- Batteries are complex, multi-scale 3D dynamical sys
- The material properties at the nano-scale affect the electrochemical properties at meso-scale and devic
- Need to develop a frame-work to integrate the mode different scales to make predictions of system-level performance and safety
- Large range of time and length scales of coupling

ed Approach

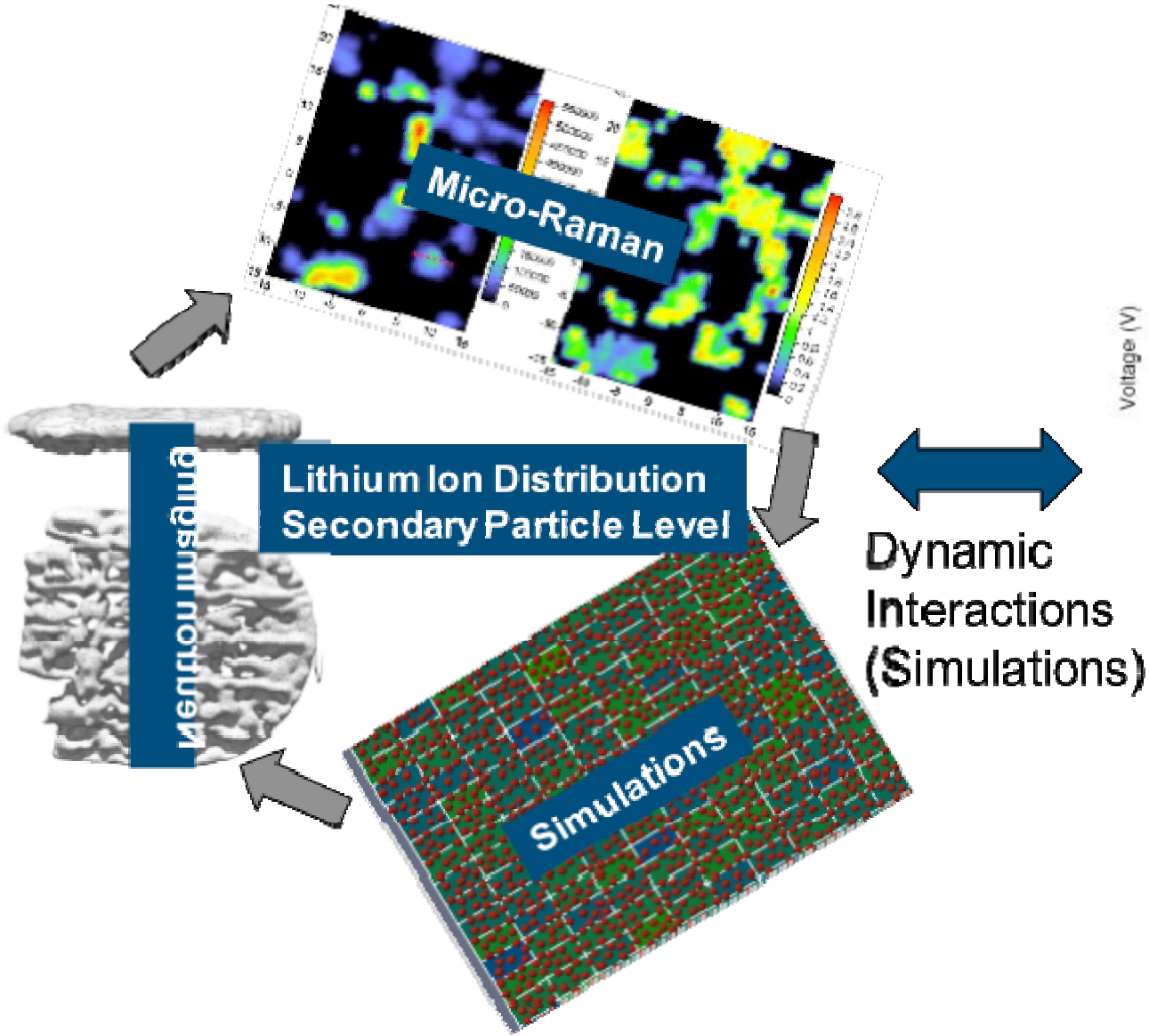
: 3D Spatio-temporal transport of charge
orous averaging techniques along with detailed
on with neutron imaging and micro-Raman
ues at the secondary-particle level
article and full cell performance interactions
2: Interfacial chemical reactions on cell performance
3: Study thermal runaway and mechanical stresses



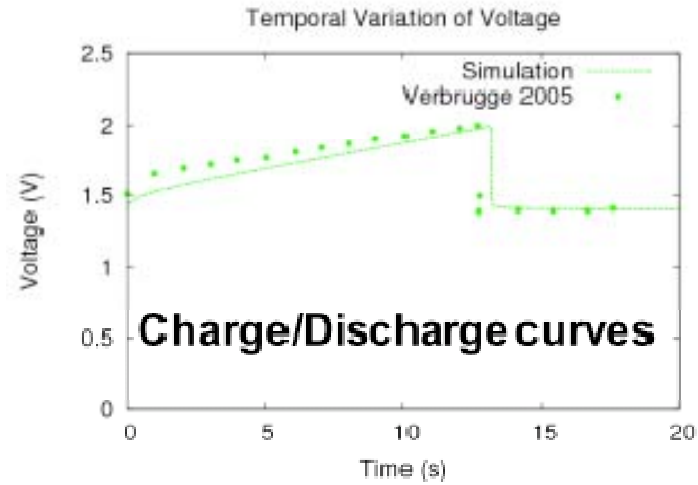
amical systems



ery model



Dynamic
Interactions
(Simulations)



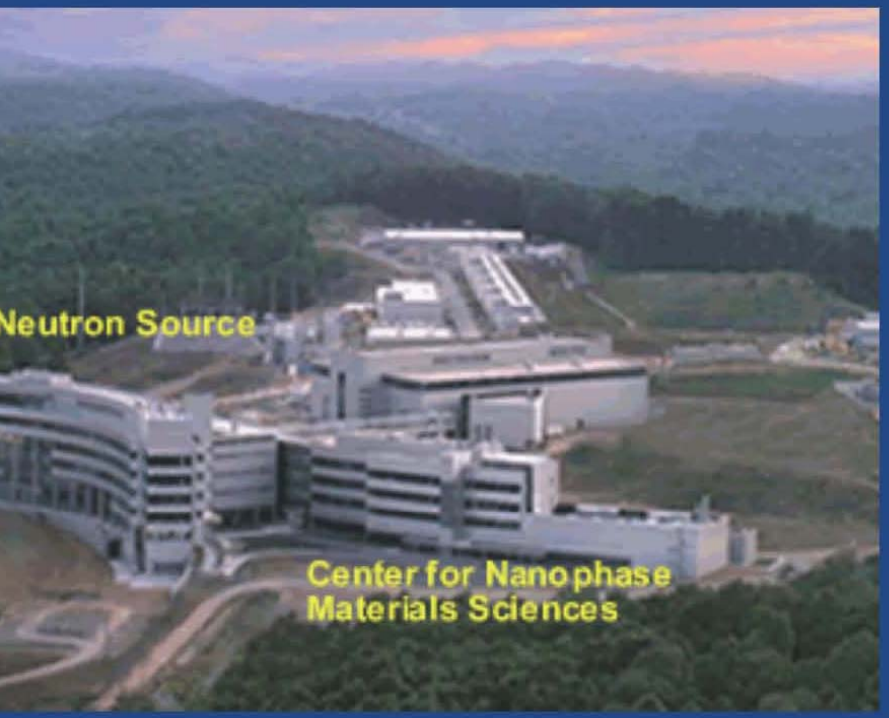
System level Performance (Cell) –
Experiments and Simulations

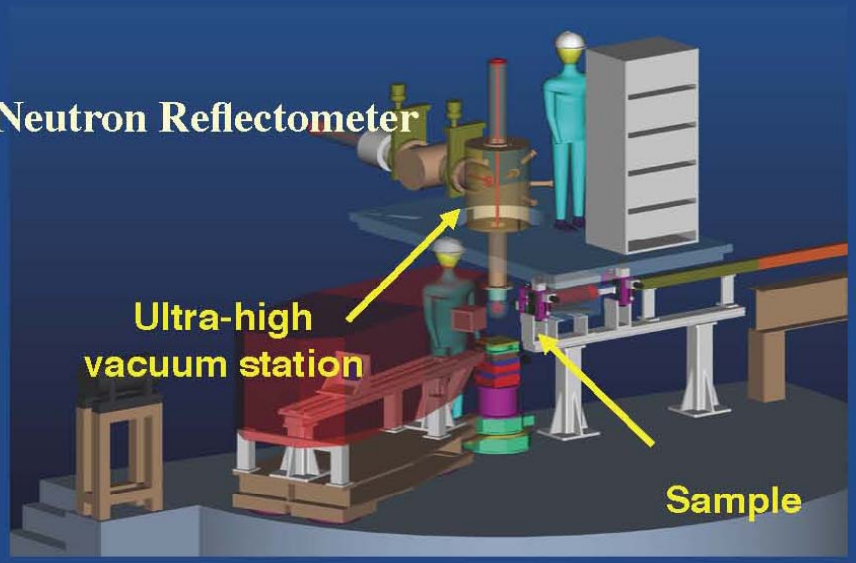
Simulations:
Dynamical spatio-temporal variations
Thermal behavior
Detailed chemistry
Mechanical stresses

ry modeling requires a multidisciplinary approach

sonnel with relevant extensive experience in theory, simulations and eriments

nbination of unique experimental and software capabilities, high-





Facility

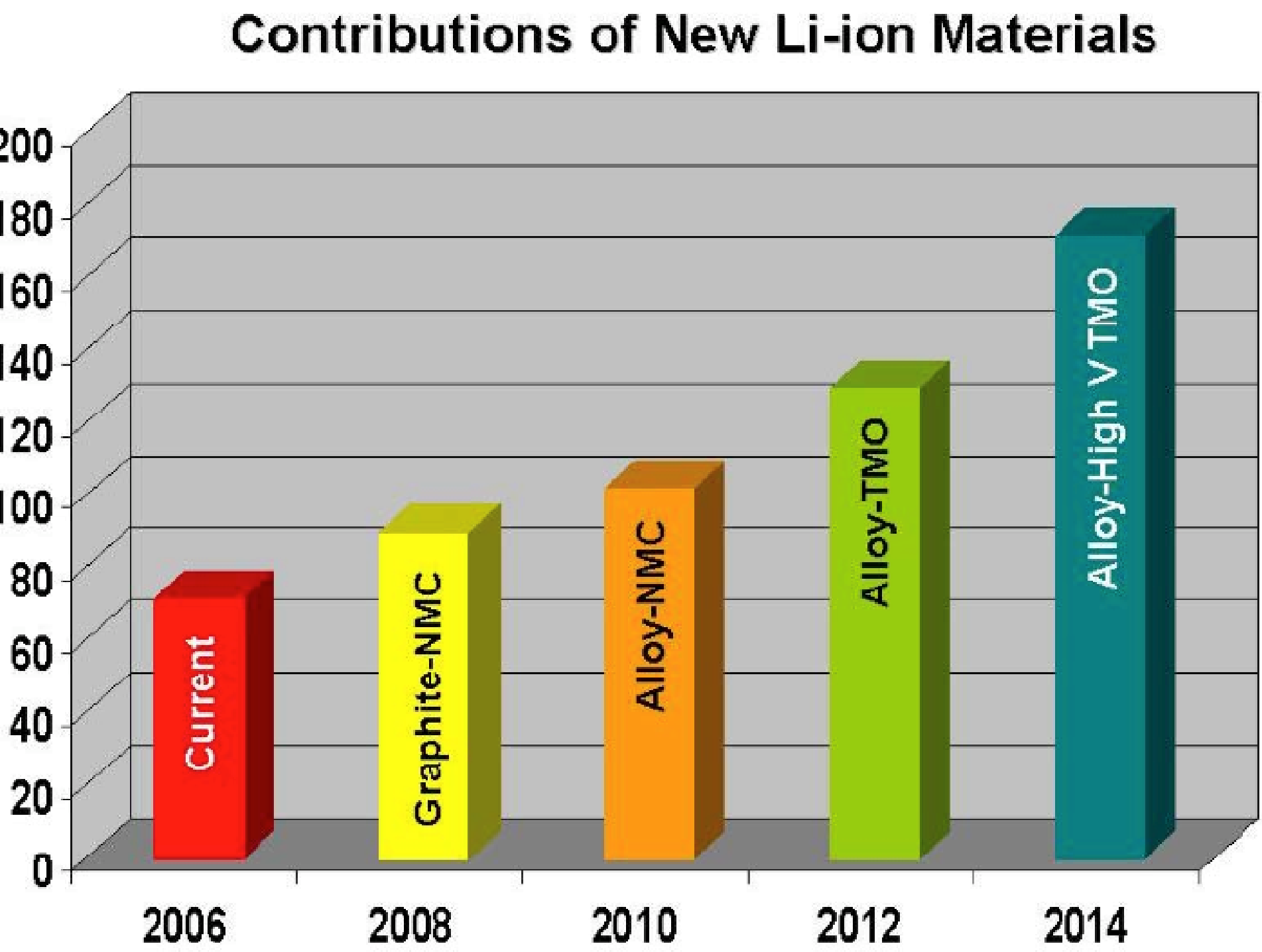
Instrumentation

Computational "Endstation" for Nano- & Materials Science

Materials, Chemistry, Physics : Math : Computer Science

- *Open Source Repository*
- *Generic Tool Kit*
- *Unified I/O systems*
- *Optimized Kernels*

batteries are only going to improve by 2



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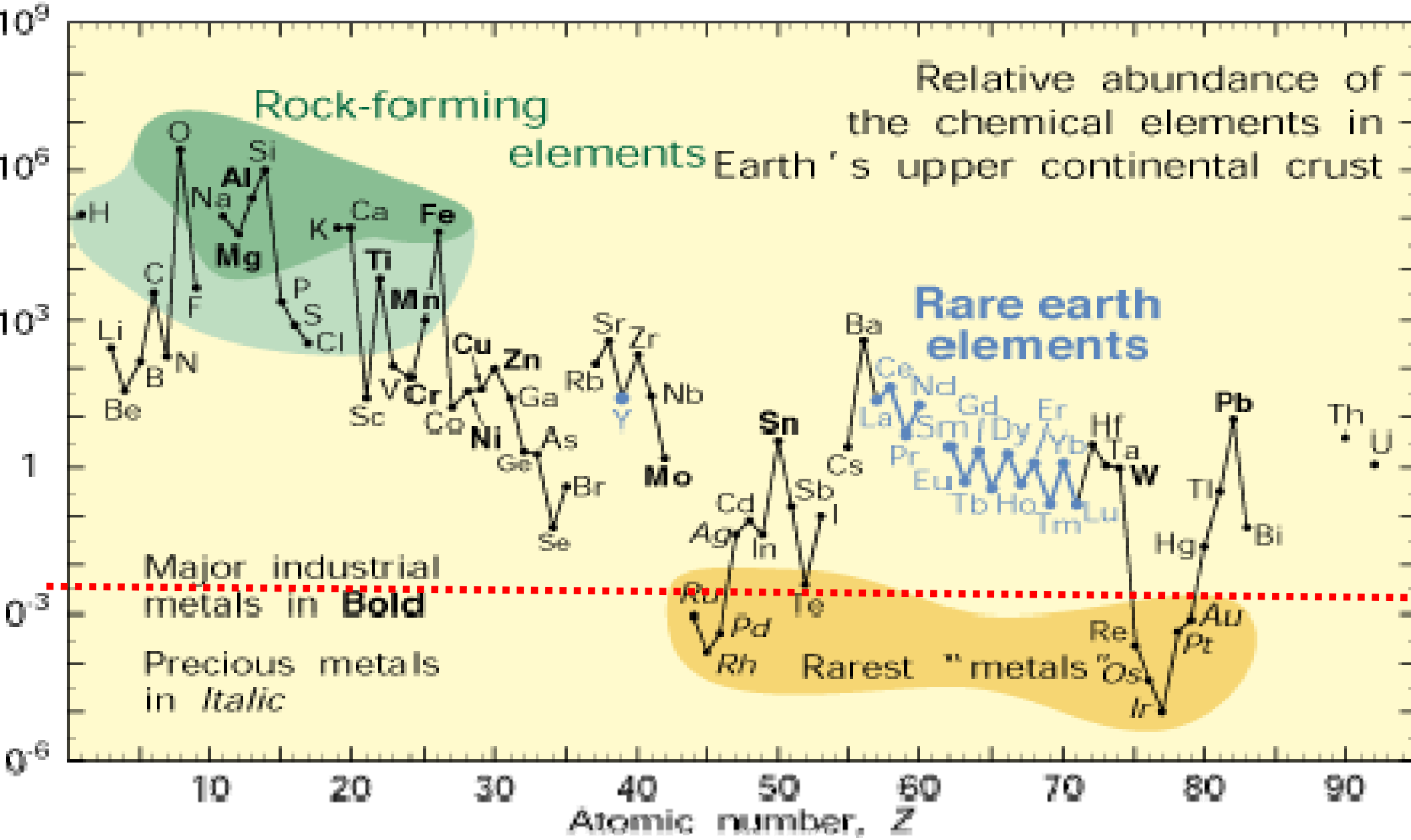
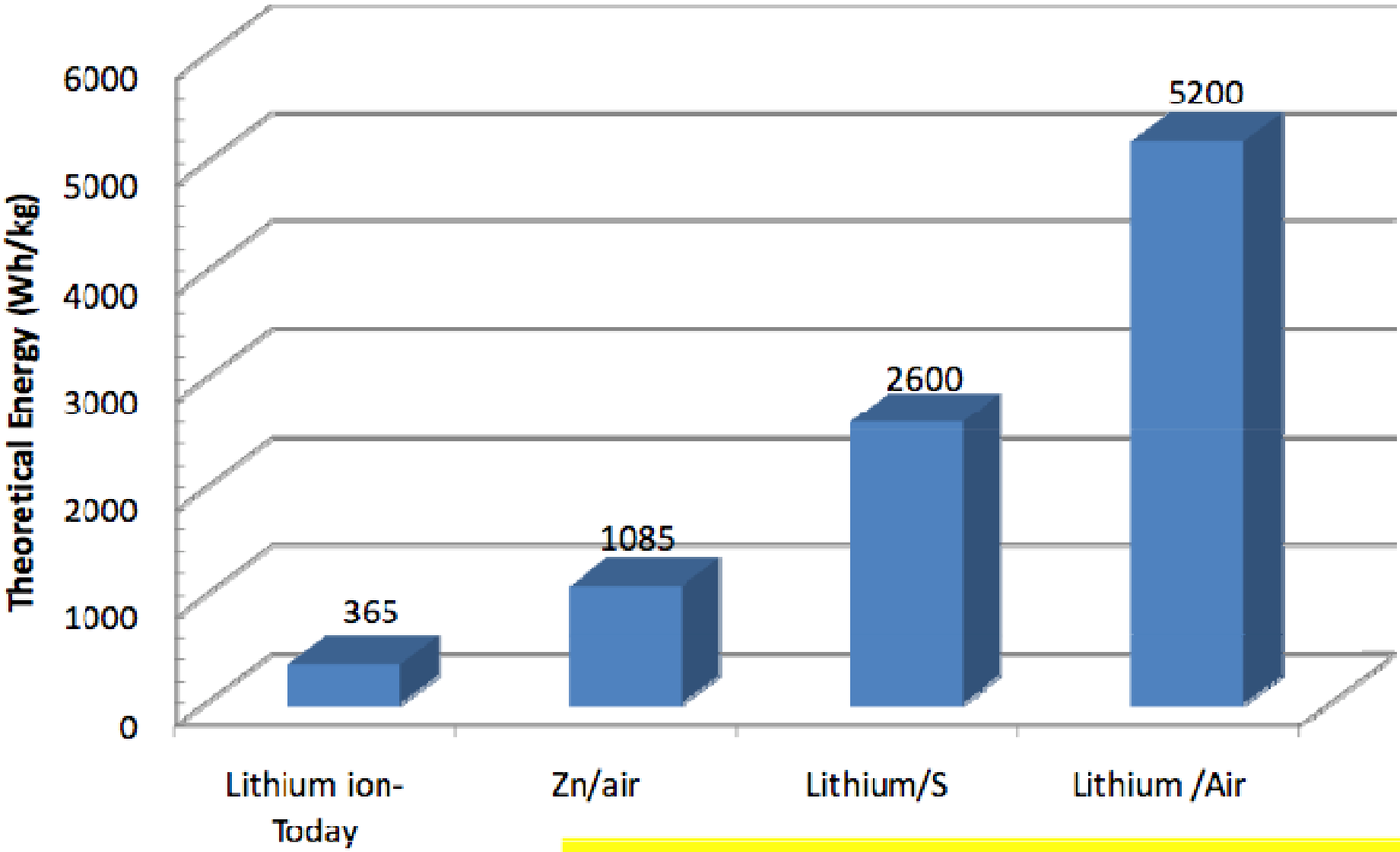


Source USGS

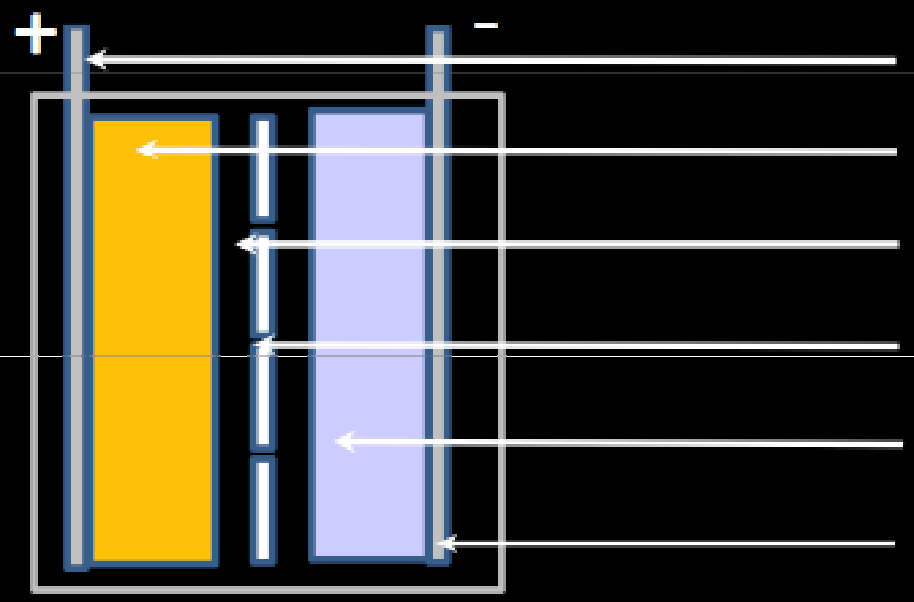


All numbers represent theoretical energy dens

stems exist that promise very high theoretical energy

wever challenges are daunting

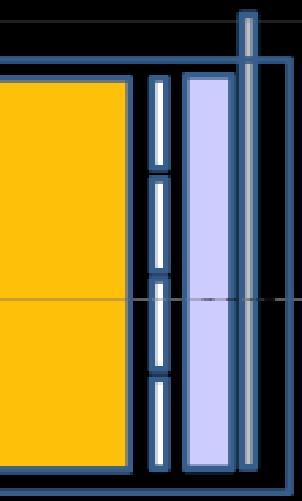
orts are underway to perform the long term research to solve these problems



(+) Current collector
Positive electrode ($LiMO_2$)
Electrolyte (alkyl carbonates
Separator (new ceramic ble
Negative electrode (graphit
(-) Current collector

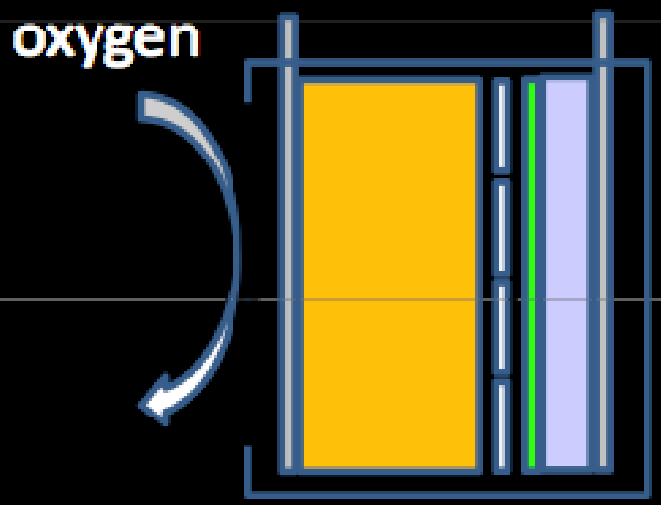
Li-ion Battery

$Li^+/e^- \leftrightarrow 2Li_2S$



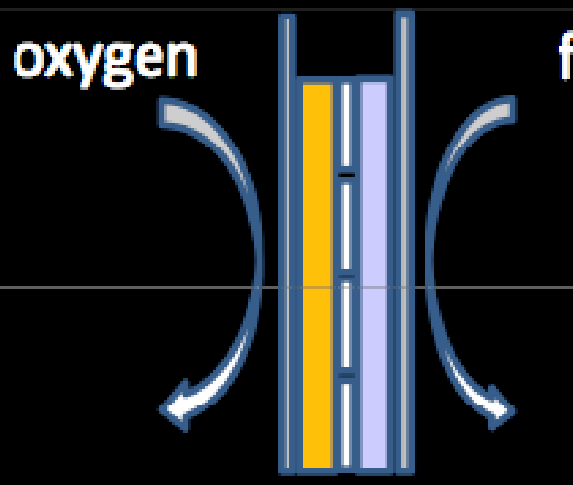
-S Battery
roduct: Li_2S

$O_2 + 2\ Li^+/e^- \leftrightarrow Li_2O_2$



Li-Air Battery
product: Li_2O_2

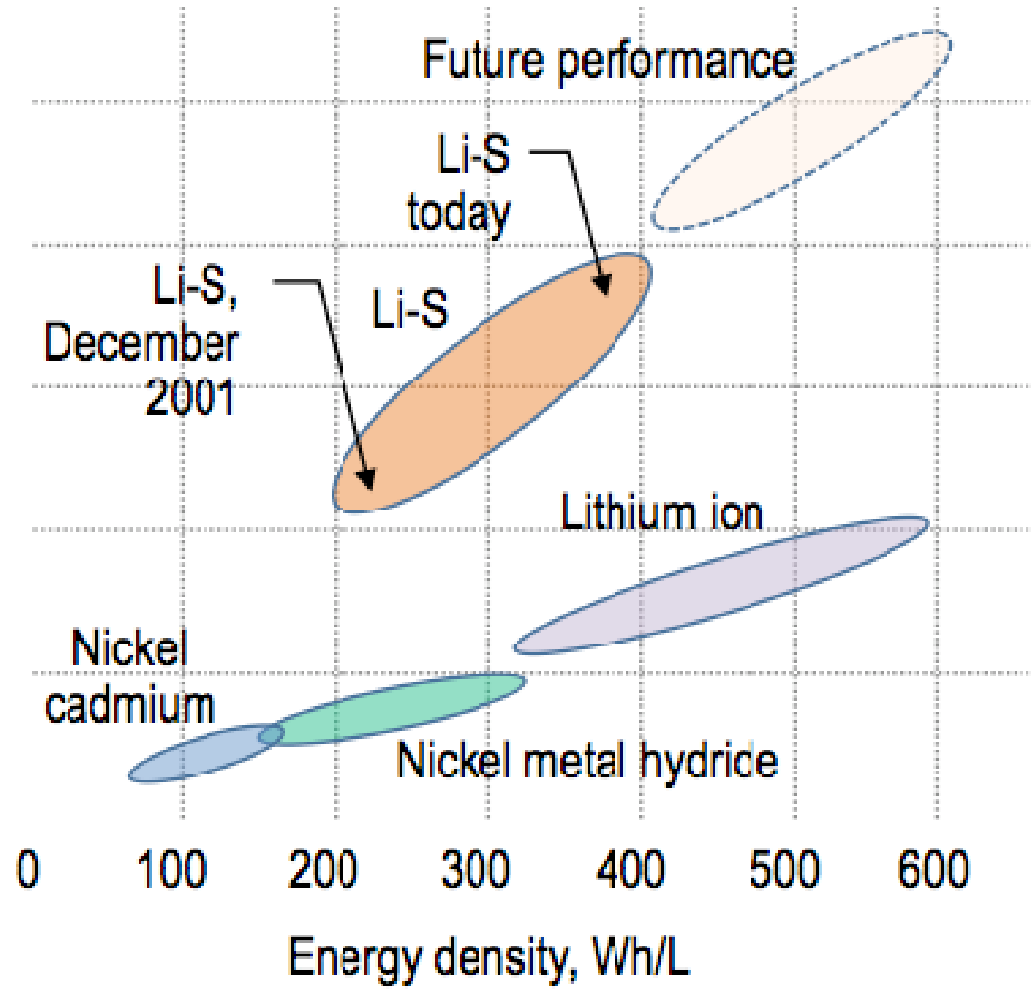
$O_2 + 4\ H^+/e^- \leftrightarrow$



Fuel Cell
Product: H_2O

e promise of lithium-sulfur

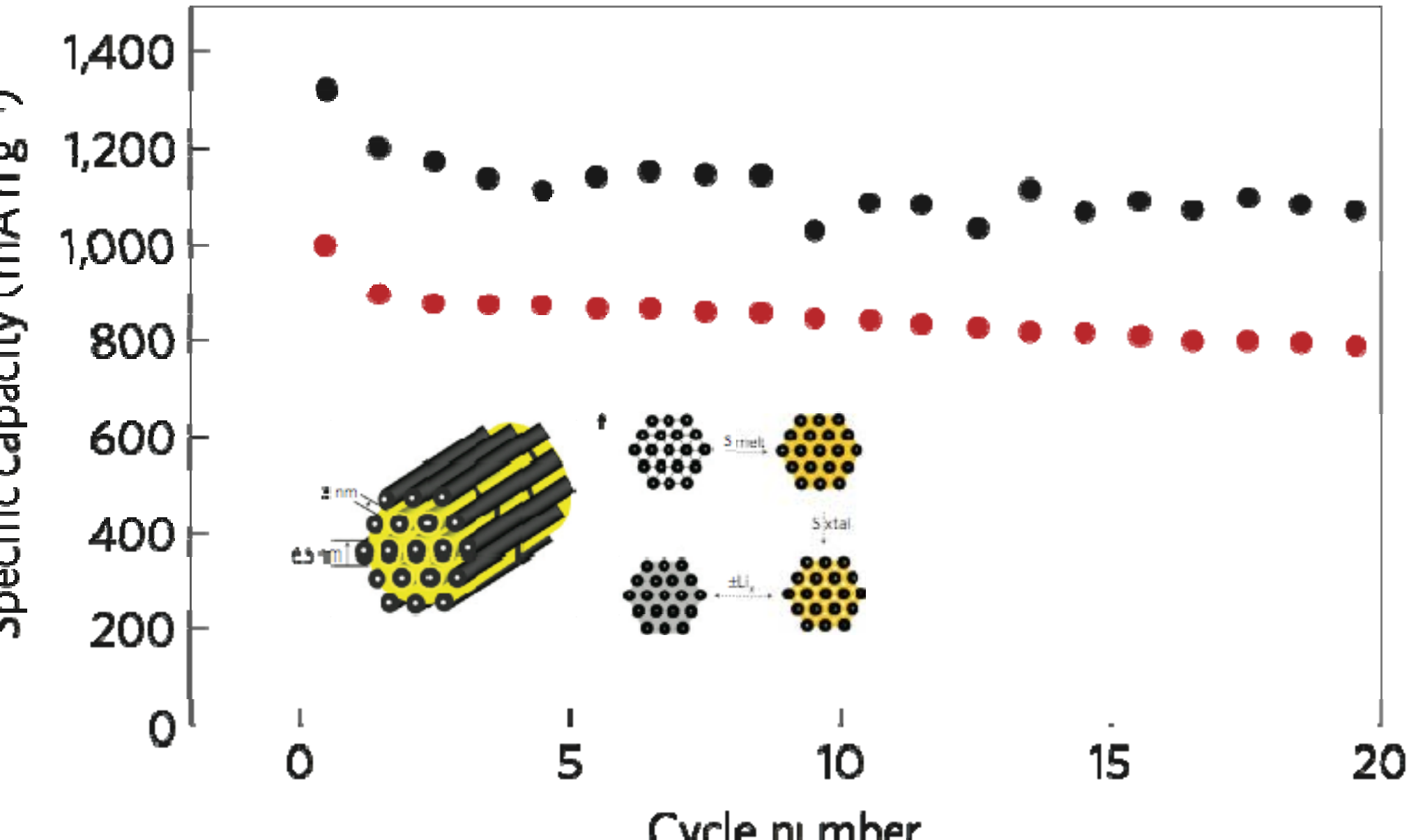
LiS is capable of 600 Wh/kg, far exceeding DOE's goal of 150 Wh/kg by 2015

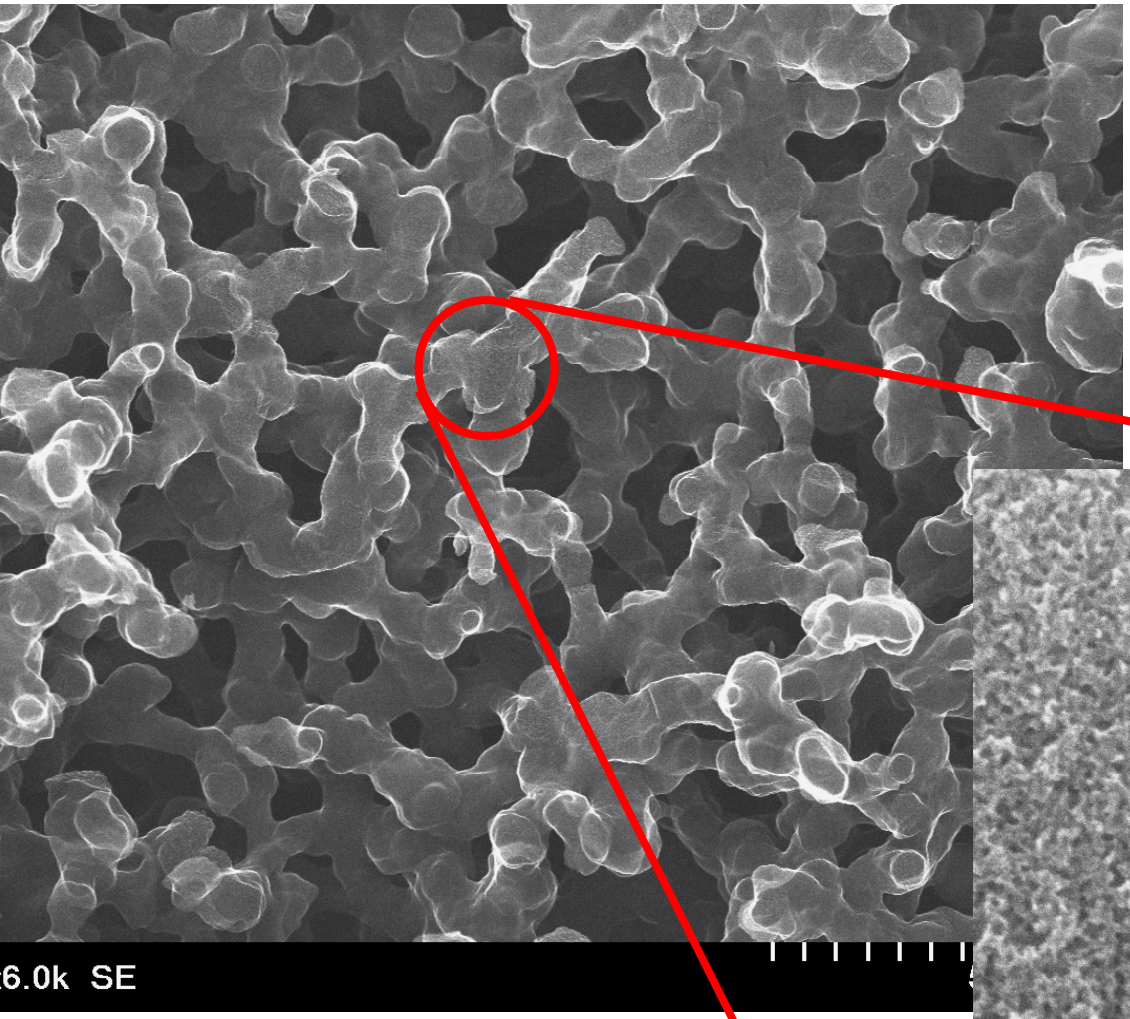


Advantages	Disadvant
• High power density • High energy density • Environmentally benign • Low cost • Safety • Excellent abuse tolerance	• Low elec conducti • Poor cyc

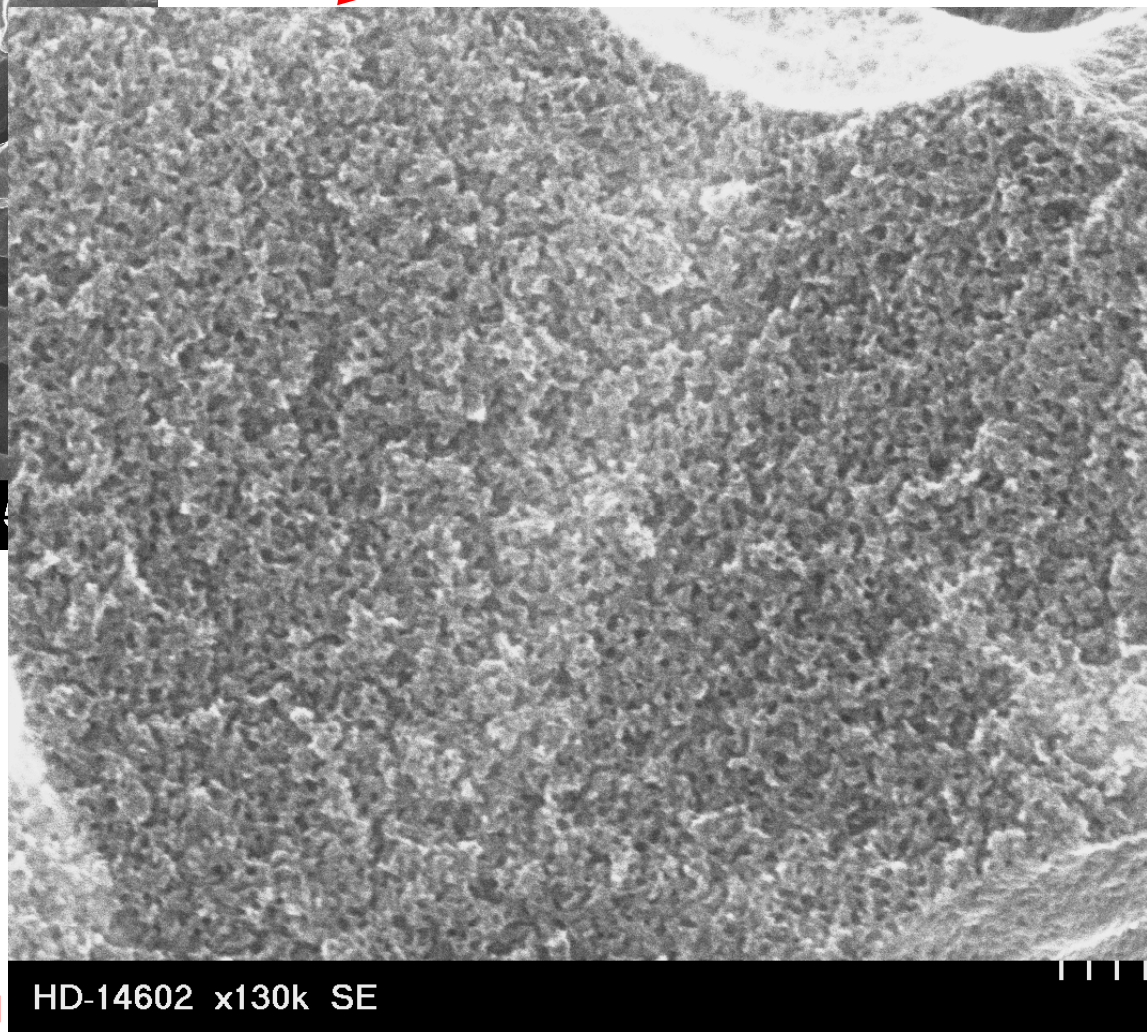
Cathode material	Theoretical capacity (mAh/g)	Voltage (V)
$LiCoO_2$	275	3.7
$LiNiO_2$	274	3.4
$LiMn_2O_4$	148	3.8
$LiFePO_4$	170	2.8
S_8	**1675**	**2.1**

oves sulphur conductivity for Li/S eries





Mesopores for nanoparticles

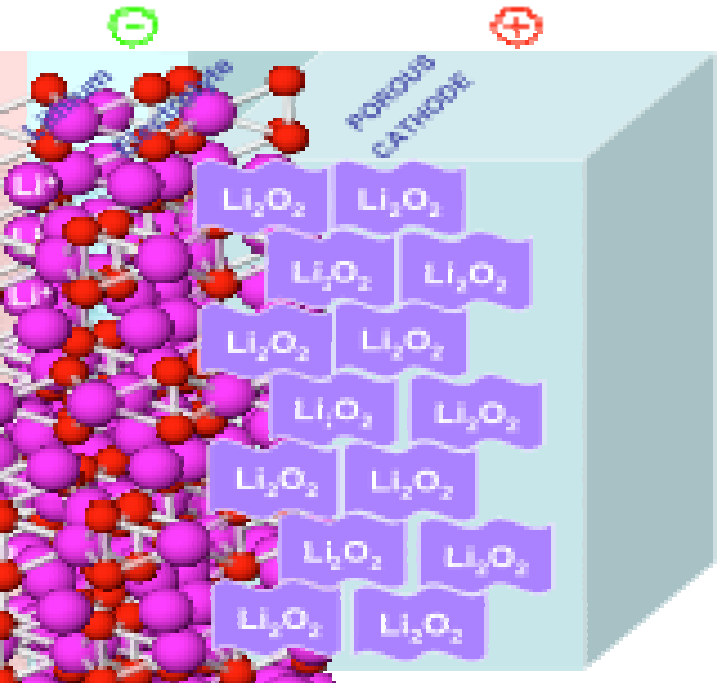


pores for electrolyte

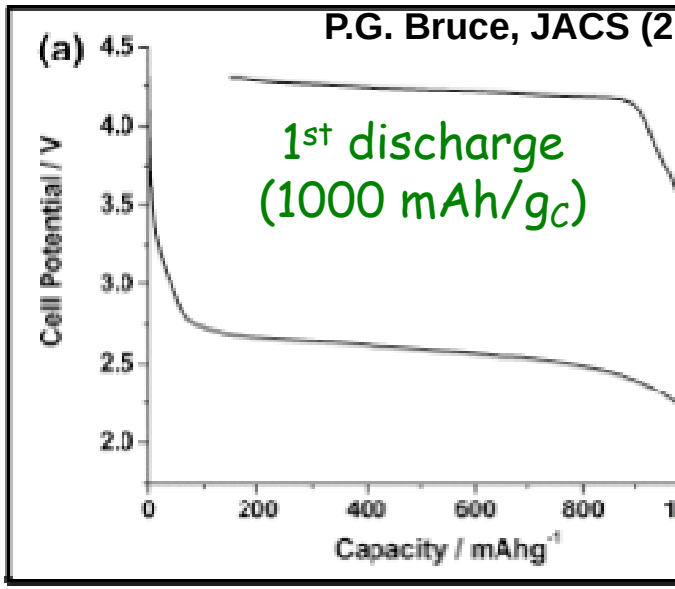
ent 20050169829: " Robust Carbon Monolith Having Hierarchical Porosity", Sheng Dai, Georg

New Materials, Chemistries and Strategies

cells: A step towards the holy grail?



Proof of concept

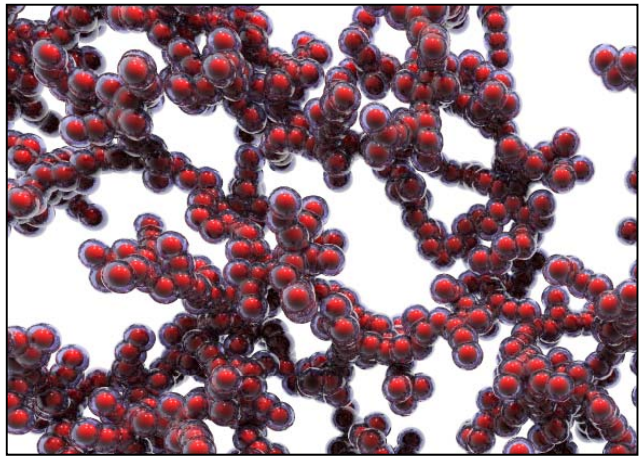


Future direction

■ Design nanomaterials to incr
capacity and power and design
functional surfaces

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

(1169 mAh/g)



Design o
catalyz
nanoarch
as air c

electrochemical couples required for
ough' improvements

igm shift away from conventional solid state

ARPA-E to advance Li-air batteries

us: Game-changing improvements

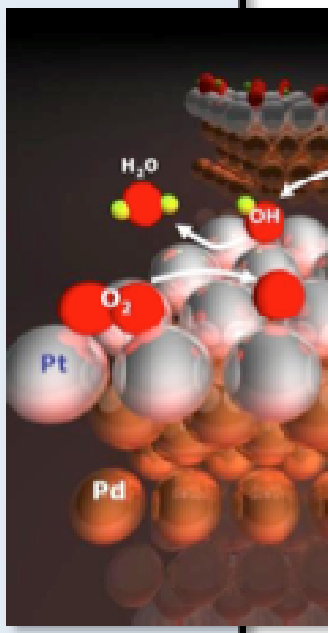
- Stretch goal: Practical energy density of 2000 Wh/kg (Li-air batteries today: 100–200 Wh/kg)
- Challenges: Power density, recharge properties, overvoltages

sed approach:

- Deep science to establish feasibility (precompetitive)
- Engineering (establish IP)
- Manufacturing

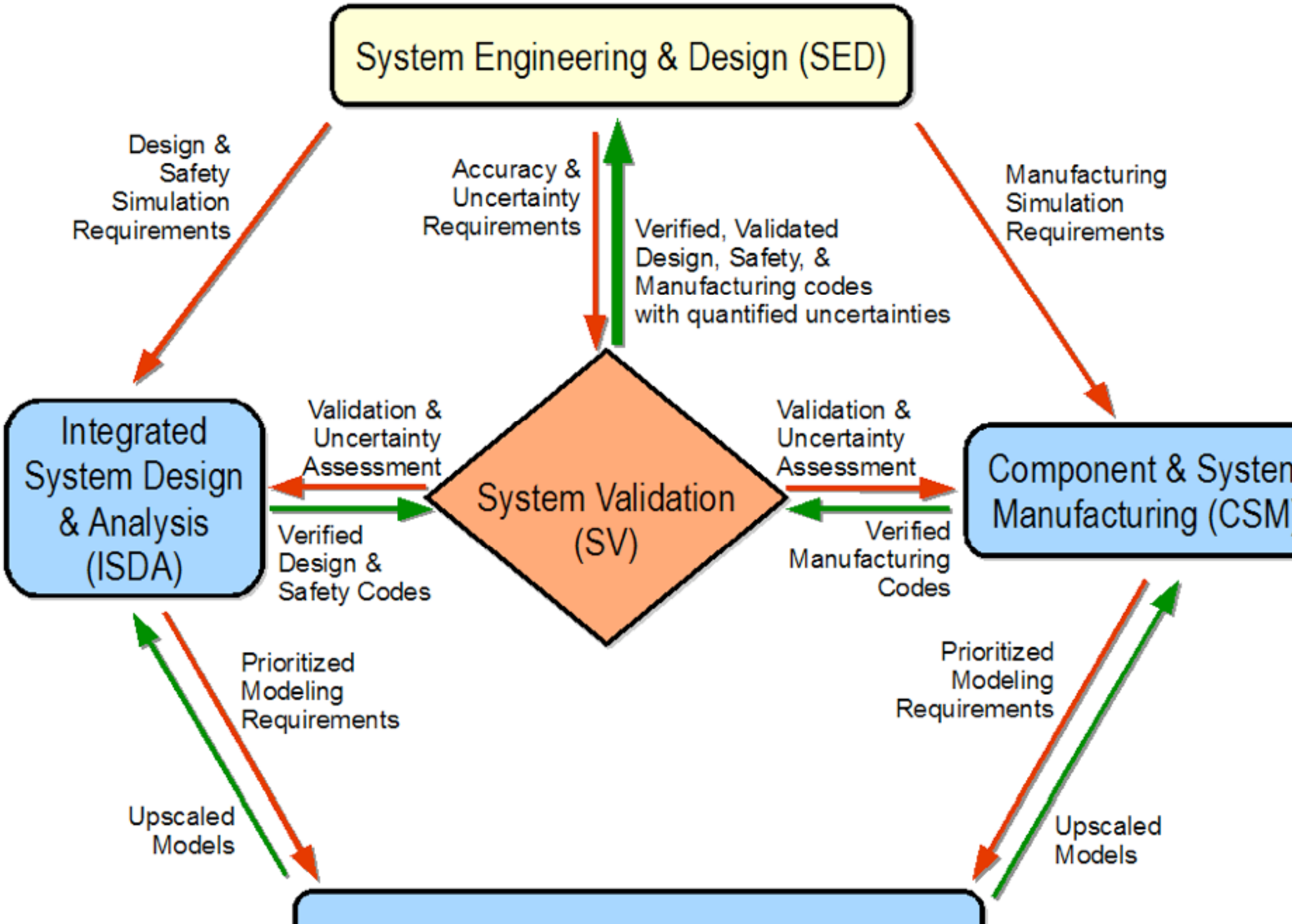
Research strategy

- **Experimental:** Exploit expertise in nanostructures, materials science, and polymers
- **Computational:** Apply supercomputing capabilities to R&D of rechargeable Li/air batteries of high power density

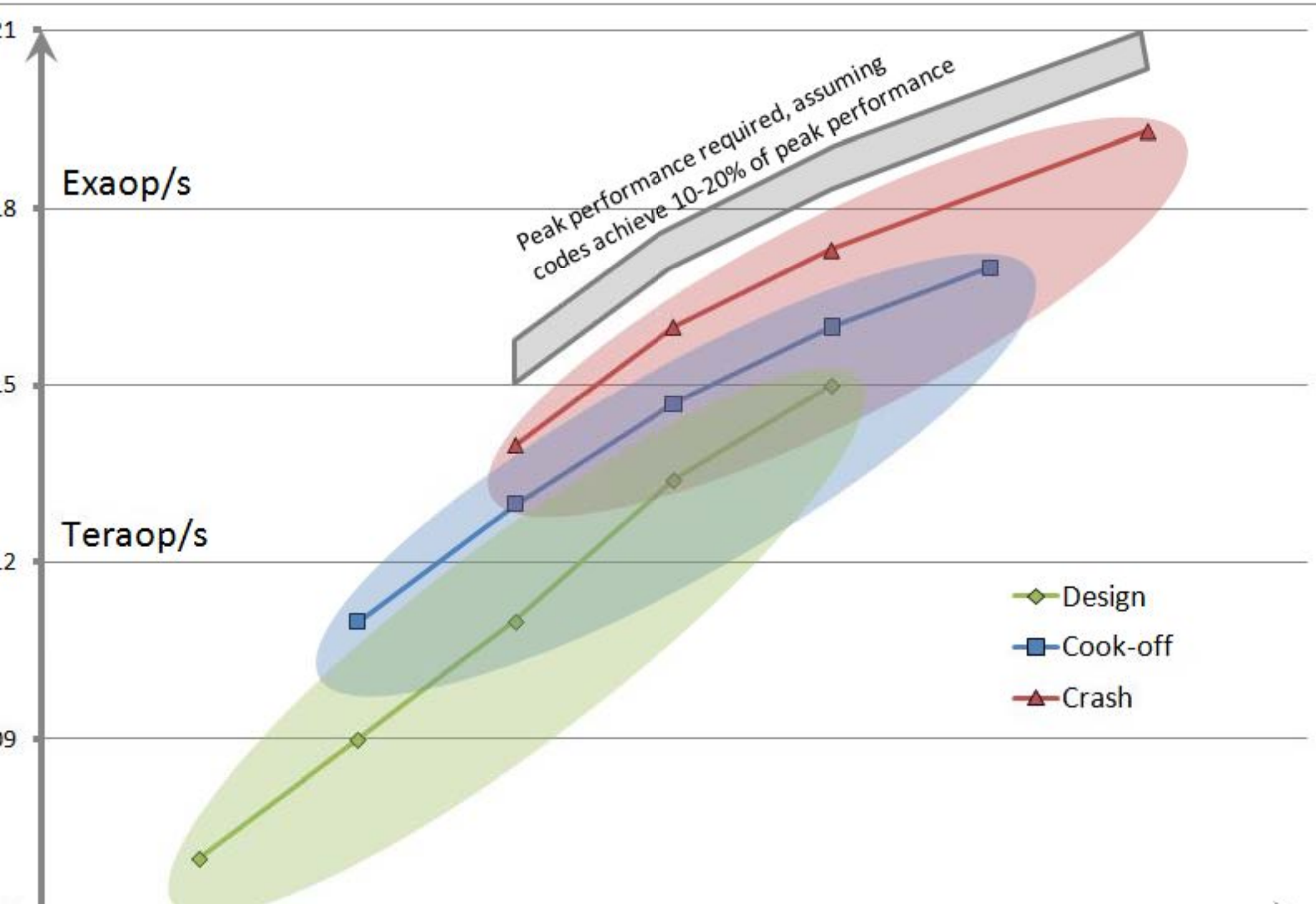


nology Review BY MIT

Thursday, June 11, 2009 IBM Invests in Battery Research The company hopes to develop powerful, lightweight lithium-air batteries.


System Engineering & Design (SED)
Design & Safety Simulation Requirements
Accuracy & Uncertainty Requirements
Verified, Validated Design, Safety, & Manufacturing codes with quantified uncertainties
Manufacturing Simulation Requirements
Integrated System Design & Analysis (ISDA)
Validation & Uncertainty Assessment
Verified Design & Safety Codes
System Validation (SV)
Validation & Uncertainty Assessment
Verified Manufacturing Codes
Component & System Manufacturing (CSM
Prioritized Modeling Requirements
Upscaled Models
Prioritized Modeling Requirements
Upscaled Models

puters


21
18
15
12
09
Exaop/s
Teraop/s
Peak performance required, assuming codes achieve 10-20% of peak performance
Design
Cook-off
Crash

akthroughs in materials are needed for ctrochemical energy storage.

mputational science, the “third-leg” of dern science, has a vital role to play in ancing innovation.

mputational science for complex materials avior is “big science”, requiring large lities and sustained support for scientific tware engineering.

h-energy battery designs, such as Li/air or , have the potential for 10x increases in