NorthEast Center for Chemical Energy Storage

http://necces.binghamton.edu

NECCES — A DOE Energy Frontier Research Center

EFRC mission statement

Develop an understanding of how key electrode reactions occur, and how they can be controlled to improve electrochemical performance, from the atomistic level to the macroscopic level throughout the life-time of the operating battery. (Focus is on intercalation electrodes and on lithium)

Internal Science Advisory Board:

Clare Grey & Gerbrand Ceder

Informal ongoing advice

Director

M. Stanley Whittingham

Associate Director

Glenn Amatucci

Formal annual review of scientific progress

External Science Advisory Board (SAB):

Bill Bushong/Rayovac, George Crabtree/ANL, Claude Delmas/Inst. of Solid State Chemistry, Linda Nazar/U. of Waterloo, Daniel Scherson/ Case Western Reserve U. & Venkat Srinivisan/LBNL

Thrust 1 Intercalation:

M. Stanley Whittingham

Understanding the intercalation material itself *(bulk material)*

Thrust 3 Cross-Cutting Diagnostics:

Karena Chapman

Develop the essential characterization tools to support Thrusts 1 and 2

Thrust 2 Electrode Transport:

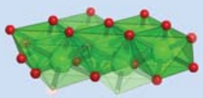
Glenn Amatucci

Understand performance limiting transport at the electrode level

Focus on in-situ and operando, National User Facilities play an essential role

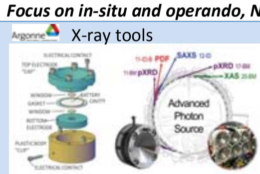
Cross-cutting characterization at all length scales

Atomic level

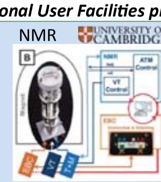


Chapman, Chupas, Argonne
XRD, PDF, XAS: AMPIX cell
Grey, Cambridge
NMR: auto-tuning probe

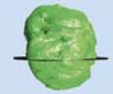
X-ray tools



NMR

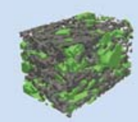


Particle level



Meng, UCSD & Cabana, UIC
Strain and chemical mapping with CXDI & X-ray microscopies
Zhou, Binghamton & Batson, Rutgers
Surface and chemically sensitive TEM

Electrode level



Grey, Cambridge
MRI
Chupas, Argonne
X-ray tomography

FIT 1.1 Beyond Olivines:

Coordinator: M. S. Whittingham

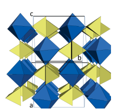
Goal 1: Attain reversible multi-electron transfer in a cathode material using lithium

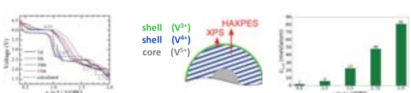
Whittingham, Chernova Binghamton — synthesis, TEM, electrochemistry

Ong, UCSD — theory

Model compound ε-Li_xVOPO_4

- ε-$LiVOPO_4$ reversibly intercalates Li
- It is a 1D diffuser
- Synthesis critical
- $VOPO_4$ reacts slowly
- Is Li_2VOPO_4 unstable?





Piper, Binghamton — spectroscopy (XPS, XAS)

Chapman, Argonne — XRD, PDF

FIT 1.2 Oxides:

Coordinator: Y. Shirley Meng

Goal 2: Close the gap between the theoretical and practical energy density for intercalation compounds

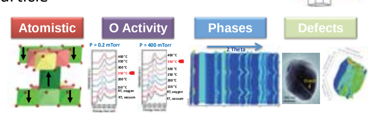
Meng, UCSD — electrochemistry, XRD, ND, CXDI

Grey Cambridge — NMR

Zhou Binghamton/ BNL — Environmental TEM

Model compound $LiNi_{0.8}Co_{0.15}Al_{0.05}O_2$ (NCA)

- 1-2% Ni on Li site.
- P_{O2} affects phase changes
- Two-phase in NCA evolving
- High defect density at single particle



Van der Ven UCSB — theory

Cabana, UIC — X-ray microscopy

Chapman Argonne — XRD

FIT 2-1: Local Level Evolution of Ionic and Electronic Transport:

Coordinator: Glenn Amatucci

FIT 2-2: Transport; mesoscale through macro:

Coordinator: Yet-Ming Chiang

Goal 3: Understand performance limiting transport in positive electrode structures from the local through the meso to the macroscale.

Amatucci, Pereira, Rutgers — sample fabrication, XRD, electrochemistry, microcalorimetry

Piper, Binghamton — surface characterization

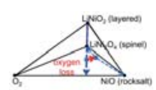
Chiang, MIT — electronic and ionic transport measurements

Thornton, Michigan — modeling across multiple length scales

Model compounds from Thrust 1: currently $LiNi_{0.8}Co_{0.15}Al_{0.05}O_2$ (NCA) and variants

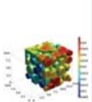
How do surface reactions induce transport issues?

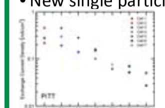
- Surface oxygen loss
  - New phases increase impedance
- Theory defining surface states
- Electrolyte is key player

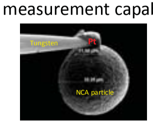


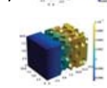
Where does impedance growth originate?

- Interfacial reaction is limiting at high SOC
- Exchange current varies by 10x at high SOC
- Meso/microscale simulations concur
- New single particle measurement capability









Ceder, UCB — theory

Batson, Cosandey Rutgers — HRTEM-EELS

U.S. DEPARTMENT OF ENERGY | Office of Science | NECCES | BINGHAMTON UNIVERSITY | RUTGERS | UNIVERSITY OF CAMBRIDGE | UC San Diego | Berkeley | UCSB | UIC | Argonne | MIT | UNIVERSITY OF MICHIGAN

This material is based upon work supported as part of NECCES, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0012583.