Probing Structure-Property Relationship of Energy Storage Materials Using Ex-Situ, In-Situ Dynamic Microscopy and Spectroscopy with High Spatial and Fast Temporal Resolution

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Purpose

- Quantitative probing of correlation of structure, chemistry, and properties of energy storage materials
- Find general guiding principle for accelerated discovery of new materials for high-density, high-power energy application
- Multimodal in-situ and ex-situ chemical imaging and spectroscopic study of structure and chemical evolution of new energy storage materials

Expected Outcomes

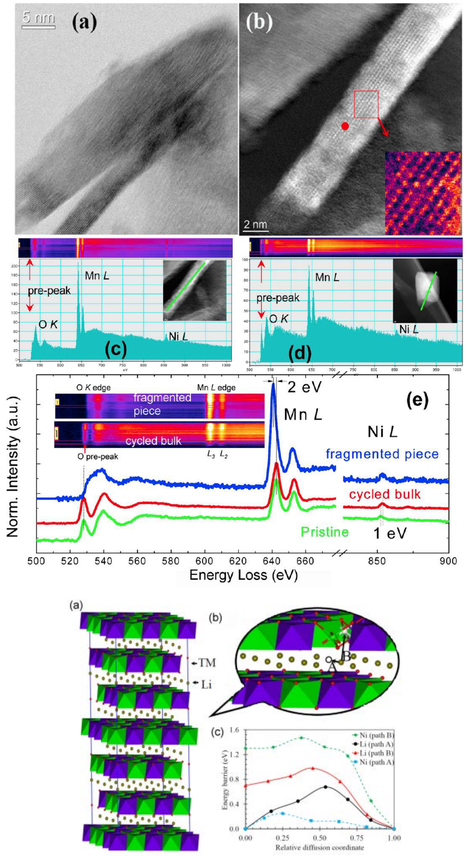
- Scientific understanding of mechanisms on capacity and voltage fading; new energy storage material development
- Understanding of electrochemical process in Li-S battery materials
- Structure-property relationship of energy materials with lattice dynamics, atomic-level chemistry, and electronic structure

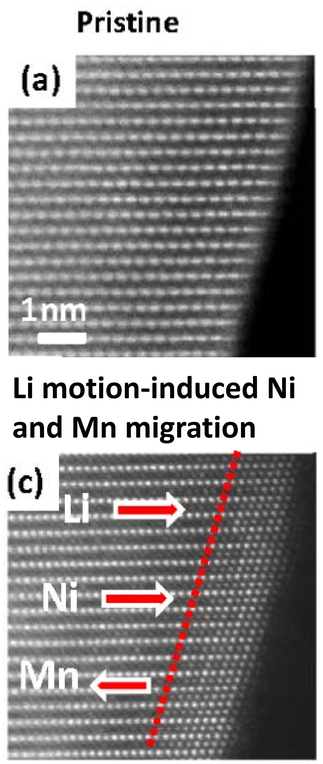
Key Successes

- Initiated fundamental concept for in-situ, atomic-level structure and chemical imaging
- Vitalized field of in-situ imaging of energy storage material structure and chemistry
- Paved critical path for chemical imaging of energy material, including JCESR, EERE-BATT characterization tasks

Research Accomplishments

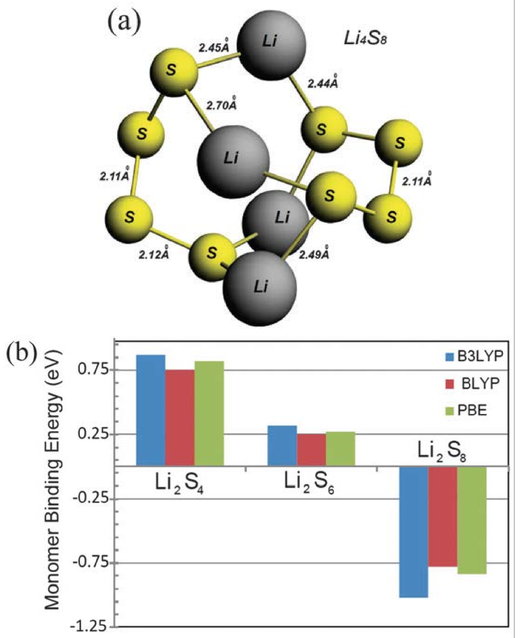
Nano- to atomic-level correlation of structure and chemistry of electrode materials for energy storage





(Gu M et al. 2013. *Nano Letters* 13:3824-3830)

- HRTEM, STEM-EELS, and computational calculation to determine structural and chemical information of $Li_{1.2}Ni_{0.2}Mn_{0.6}O_2$ and phase transformation
- Scientific understanding of the "bottleneck" on charge/discharge rate and voltage fading of lithium ion battery.



(a) Molecular structure of Li_4S_8.
(b)Binding-energy difference between the monomer and dimer units of lithium polysulfide species
(Vijayakumar et al. 2014. *PCCP* 16:10923-10932)

References and Publications

- Zheng J et al. 2014. *Nano Letters* 14:2628-2635
- Zhou J et al. 2014. *RSC Advances* DOI:10.1039/C4RA01332
- Gu M et al. 2014. *Scientific Report* 4:3684
- Gu M et al. 2013. *Nano Letters* 13:6106-6112
- Genc A et al. 2013. *Ultramicroscopy* 131:24-32
- Vijayakumar M et al. 2014. *PCCP* 16:10923-10932

Next Steps

Scientific research

- Atomic-level chemical and structural evolution and correlation with properties
- Integration of STXM and XAS ability with ex-situ, in-situ TEM, STEM, and DTEM to image complex hierarchical nanostructures used in Li-S and multivalence ions
- Tackling grant challenge in Li-ion battery field: formation, structure, chemical composition, dynamics of SEI layer
- Obtain DTEM images and diffraction for in-situ electrochemical cell with fast temporal resolution.

Programmatic Development

- Coupled to JCESR for Energy Storage
- Grow EERE-BATT portfolio to probe battery failure mechanism
- BES proposal on molecular-level materials design.