Using Unique Capabilities Of NSLS-II Beamlines (XPD, ISS, HXN, and TES) To Study Battery Materials

Enyuan Hu, Seongmin Bak, **Xiao-Qing Yang,** Xiqian Yu, Yongning Zhou, and Hung Sui Lee
Brookhaven National Laboratory, Upton, NY 11973, USA

To be presented at BNL-MIT Workshop
Brookhaven National Laboratory, July 25, 2017

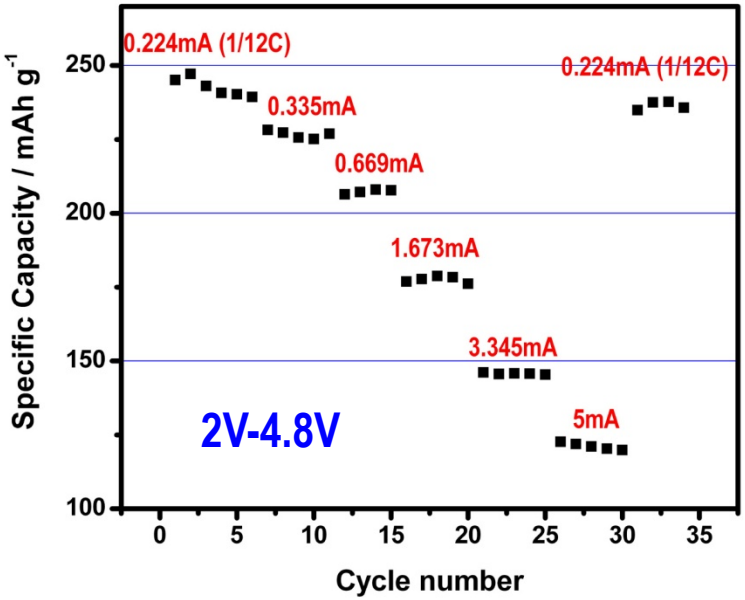
The work at BNL was supported by the Assistant Secretary for Energy Efficiency and Renewable Energy, Office of Vehicle Technologies of the U. S. Department of Energy under Contract Number DE-SC0012704

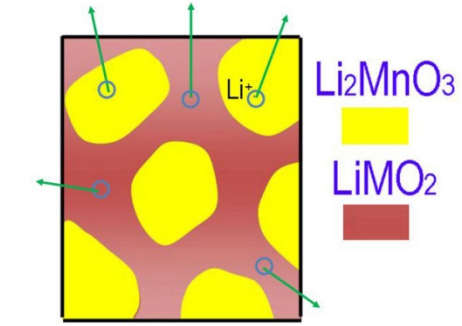
BROOKHAVEN
NATIONAL LABORATORY

Delithiation Kinetics- Time resolved XAS

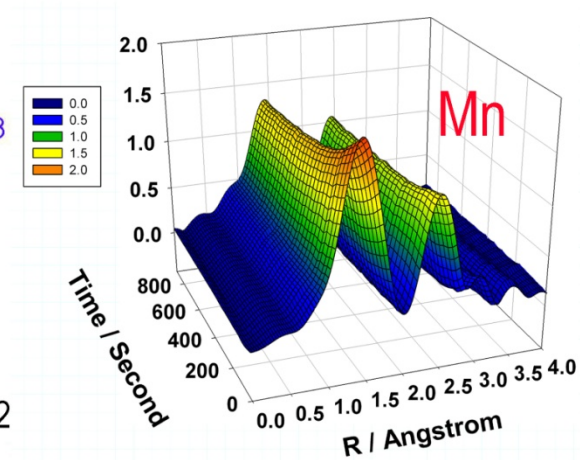
Comparing the contribution of Ni, Co, Mn to the rate capability

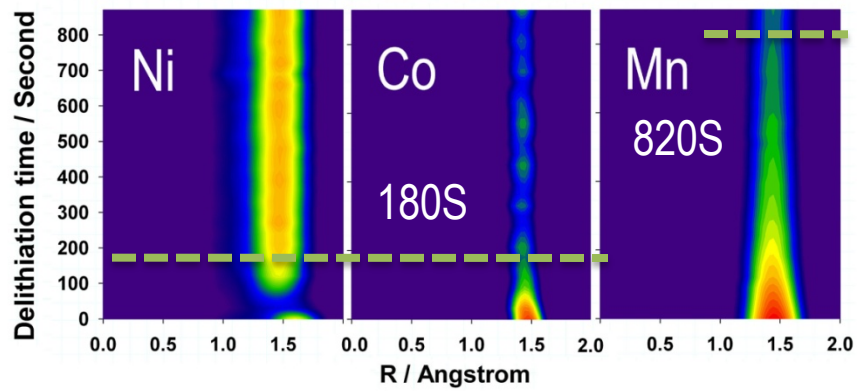
Rate performance





$Li_{1.2}Ni_{0.15}Co_{0.1}Mn_{0.55}O_2$





(1) $Li_{1.2}(Ni_{0.15}Co_{0.1}Mn_{0.55})O_2$ shows unsatisfied rate performance;

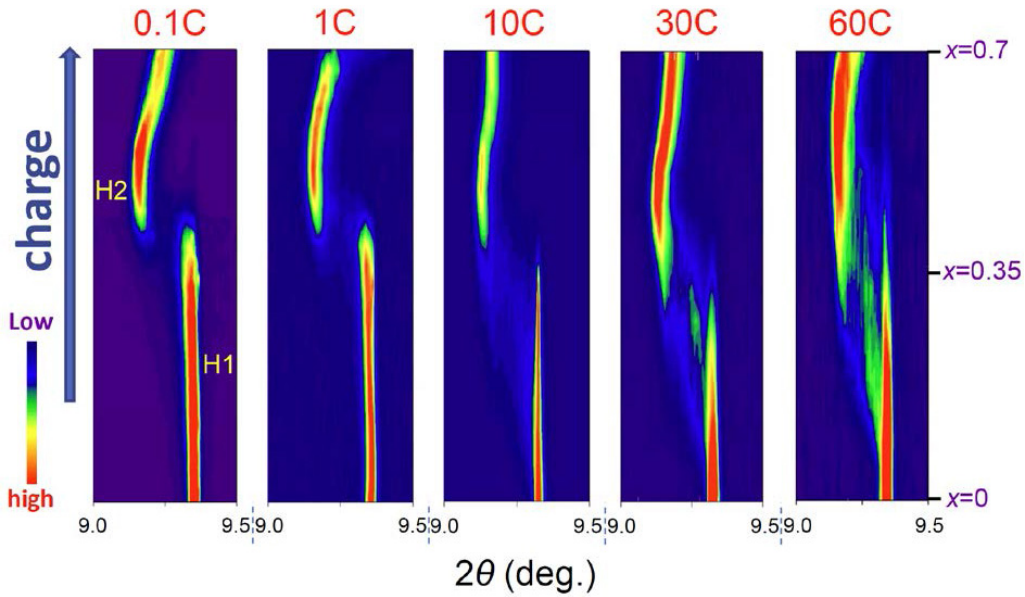
(2) Sluggish delithiation kinetic of Li_2MnO_3 component.

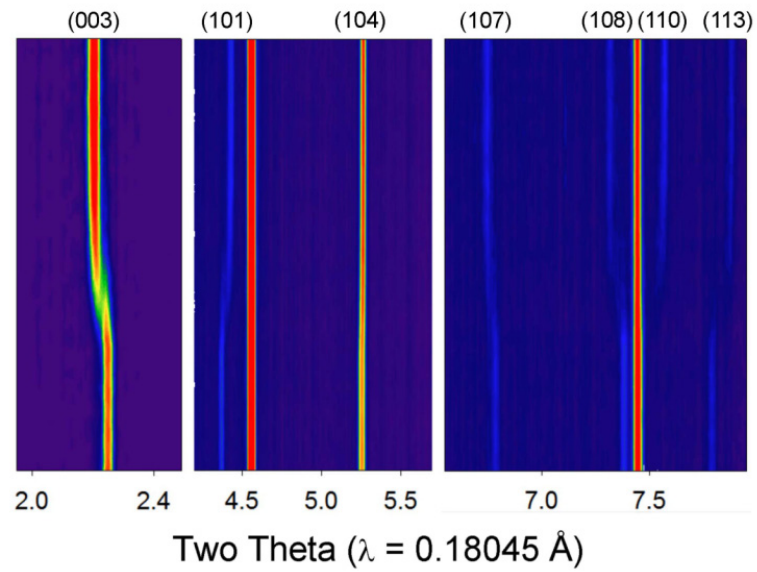
4.8V constant voltage charging, Ni, Co, Mn react simultaneously

Xiqian Yu *et. al.*, ***Adv. Energy Mater.***, (April 2014), DOI: 10.1002/aenm.201300950,

In situ XRD of NMC during the first charge. Contour plot of the (003) diffraction peak of $Li_{1-x}Ni_{1/3}Co_{1/3}Mn_{1/3}O_2$

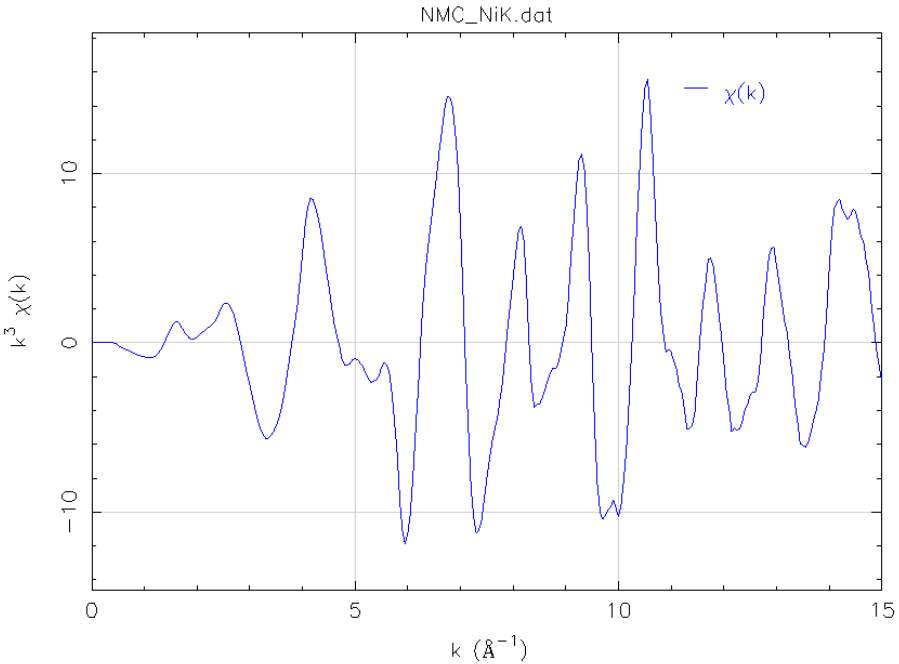
Rate performance

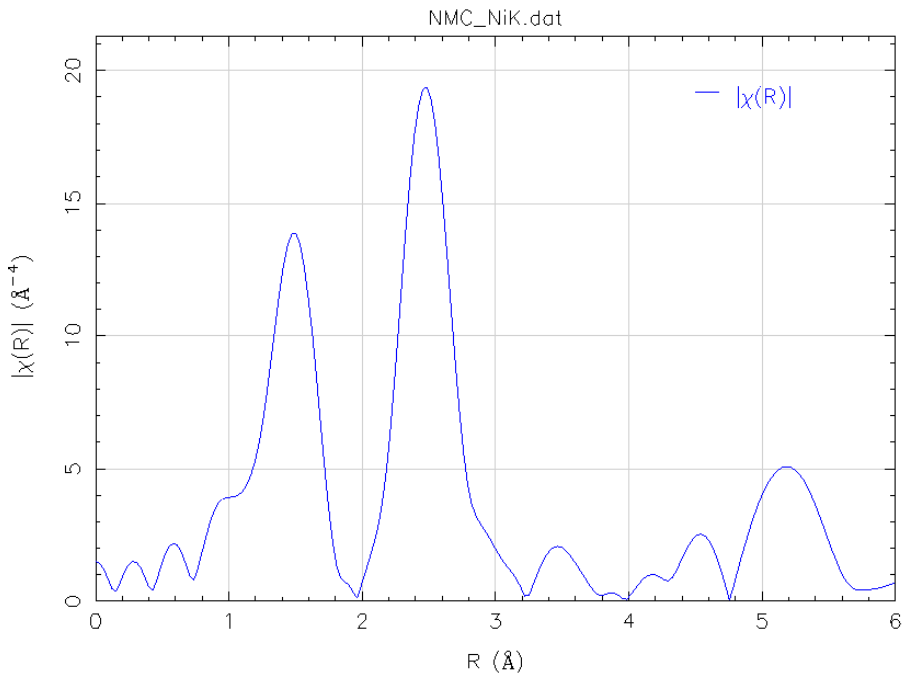




Data collected at X14A beamline of NSLS. Results published in paper by
Yongning Zhou *et. al.*, ***Adv. Energy Mater.***, (August 2016)
DOI: 10.1002/aenm.201600597

Full spectra collected at XPD beamline of NSLS-II during 60C high rate charging

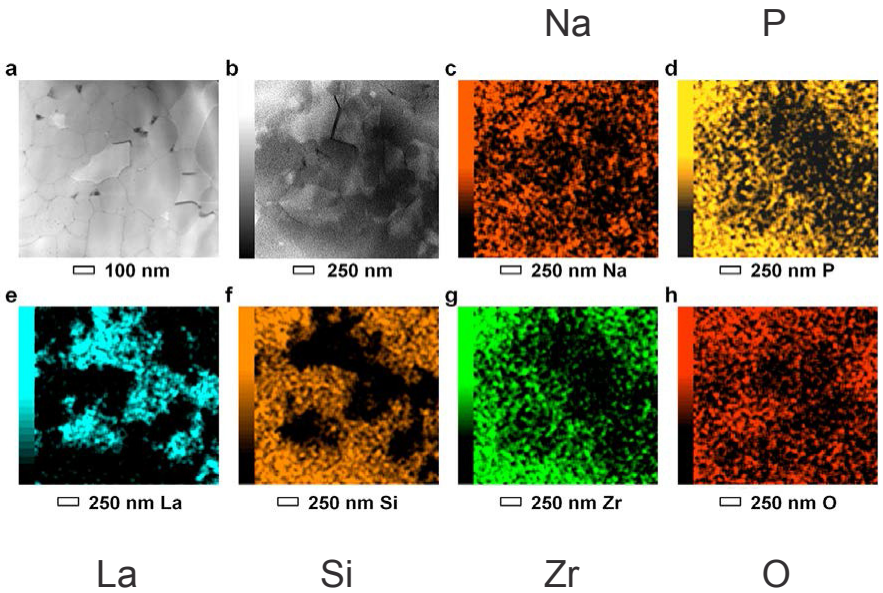




This is a 12 second XAS spectra collected at ISS beamline of NSLS-II on a high energy battery cathode material—$LiNi_{0.6}Mn_{0.2}Co_{0.2}O_2$, noted as High Ni content NMC.

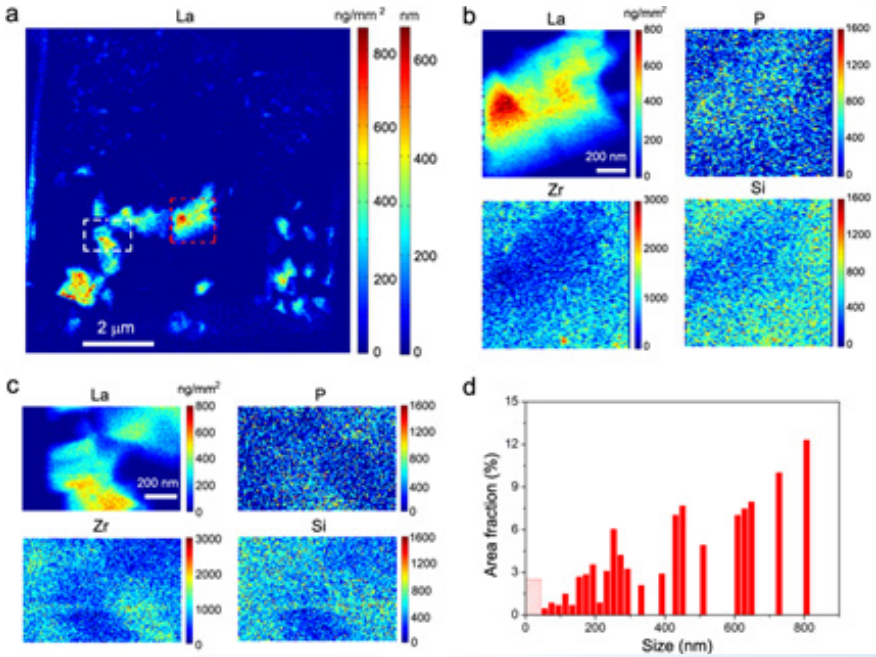
The photo of Nano-probe x-ray microscope
At Hard x-ray Nano-probe beamline (HXN) at NSLSII

Two phases of $Na_3Zr_2Si_2PO_{12}$ and $Na_3La(PO4)_2$



The microstructure of the self-formed composite solid electrolytes. (a) TEM image of nominal composition $Na_{3.15}La_{0.15}Zr_{1.85}Si_2PO_{12}$ ceramic. (b) TEM image of nominal composition $Na_{3.3}Zr_{1.7}La_{0.3S}Si_2PO_{12}$ ceramic. (c) Sodium, (d) Phosphorus, (e) Lanthanum, (f) Silicon, (g) Zirconium, and (d) Oxygen elemental mappings of nominal composition $Na_{3.3}Zr_{1.7}La_{0.3}Si_2PO_{12}$ composite electrolyte.

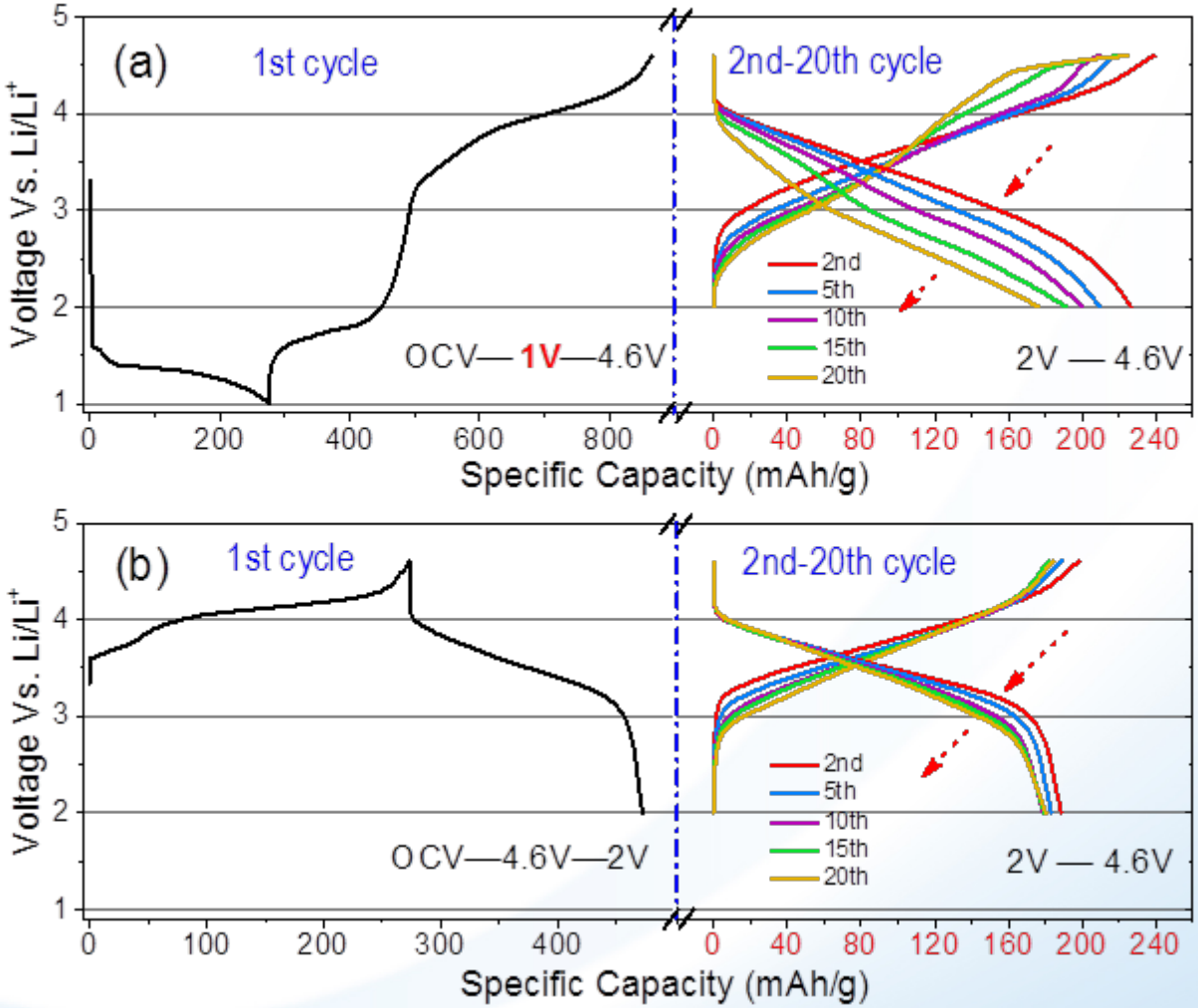
The images of elemental distribution for a novel solid-state electrolyte ceramic material sample collected at Hard x-ray Nano-probe beamline (HXN) at NSLS-II



Results published on advanced Energy Materials:

Zhizhen Zhang *et al.*, “A self-forming composite electrolyte for solid-state sodium battery with ultra-long cycle life” Advanced Energy Materials, (October, 2016), DOI: 10.1002/aenm.201601196

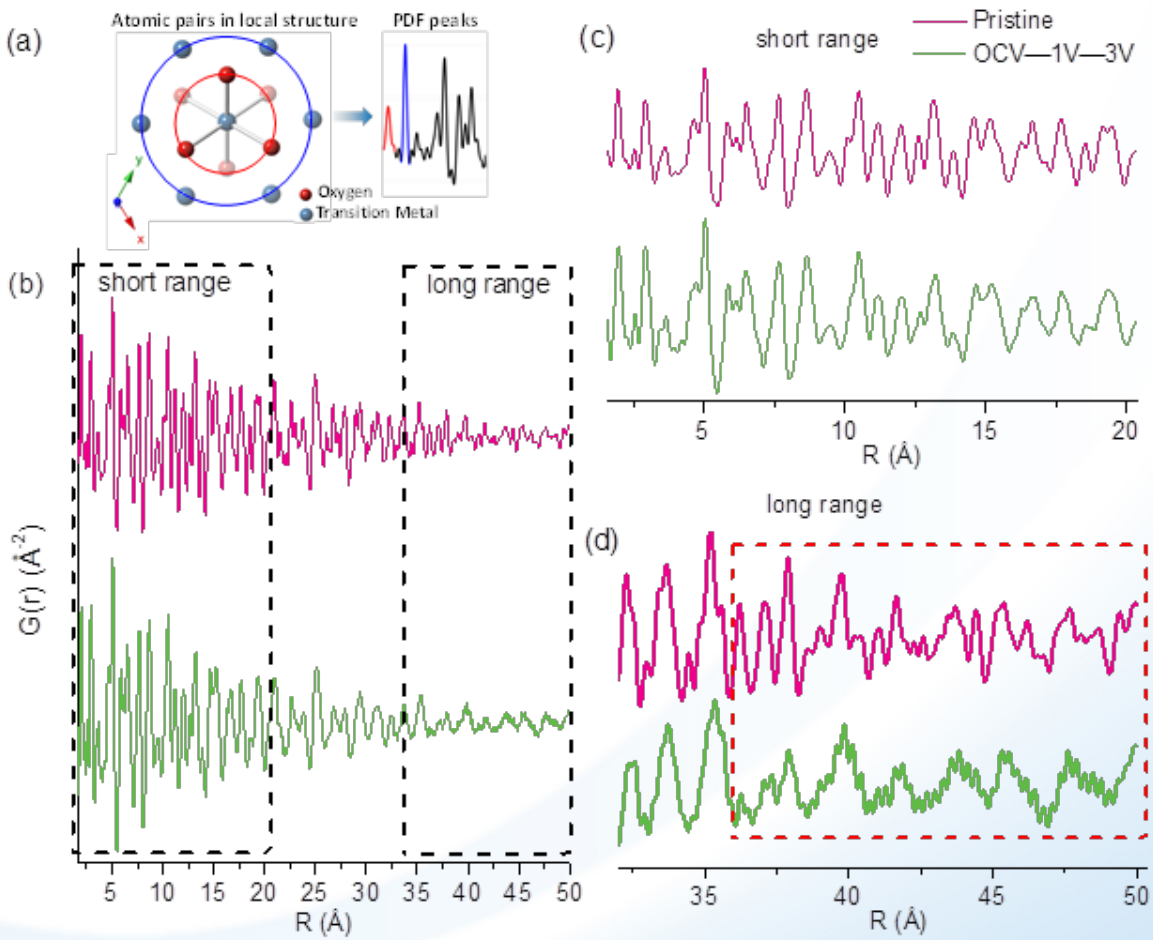
Electrochemical performances of (a) prelithiated $Li_2Ru_{0.5}Mn_{0.5}O_3$ which is first discharged to 1 V and then charged to 4.6 V, followed by cycling between 2V and 4.6 V; (b) normally cycled $Li_2Ru_{0.5}Mn_{0.5}O_3$ which is directly cycled between 2 V and 4.6 V without discharging



Enyuan Hu *et. al.*, Nano Letters, (September 2016)
DOI: 10.1021/acs.nanolett.6b01609

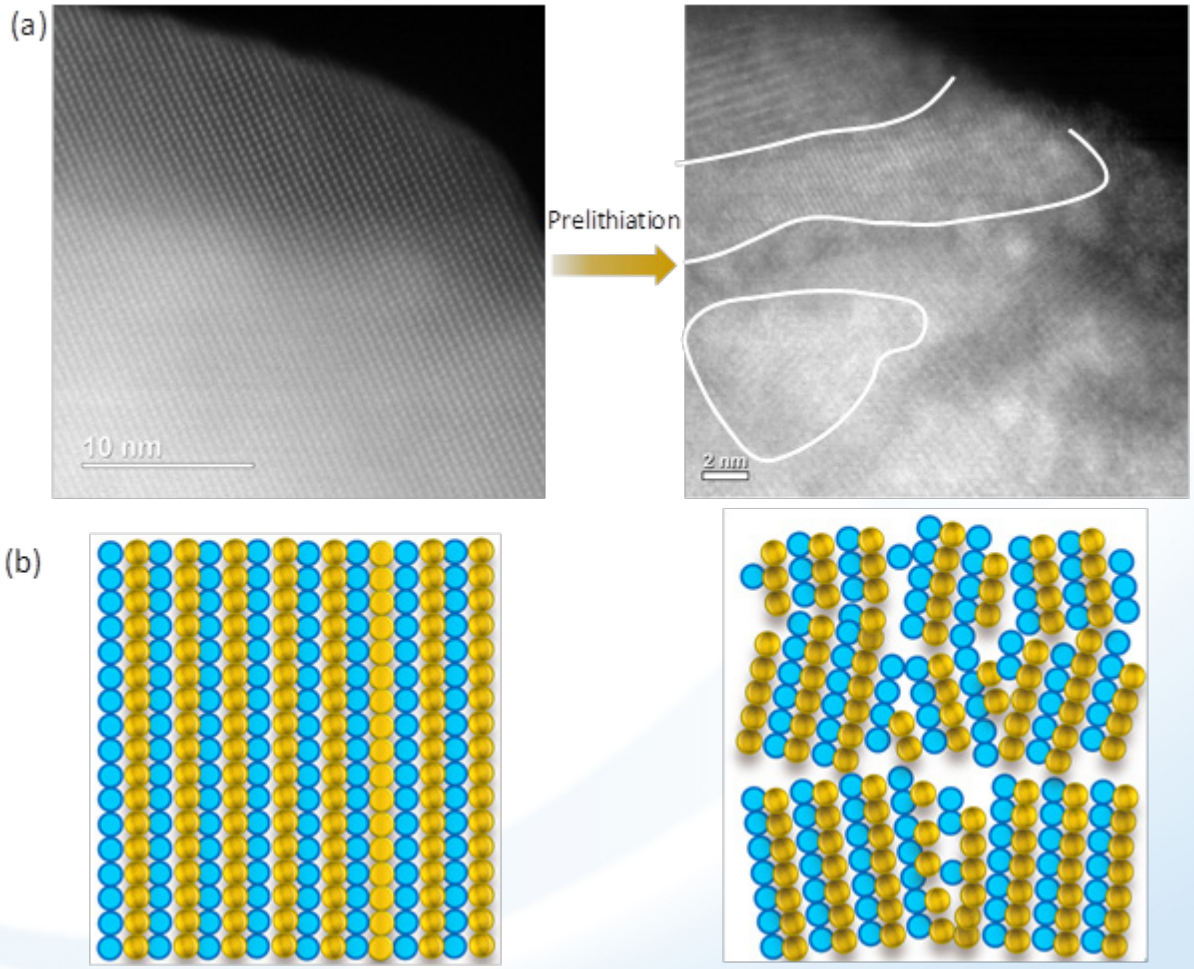
a) Illustration of PDF showing that peaks correspond to characteristic bond lengths.
b) *Ex situ* PDF data of pristine sample and "OCV—1V—3V" sample
c) zoomed in data on the short range region of ex situ PDF data and
d) zoomed in data on the long range region of *ex situ* PDF data.

Data collected at XPD beamline of NSLSII



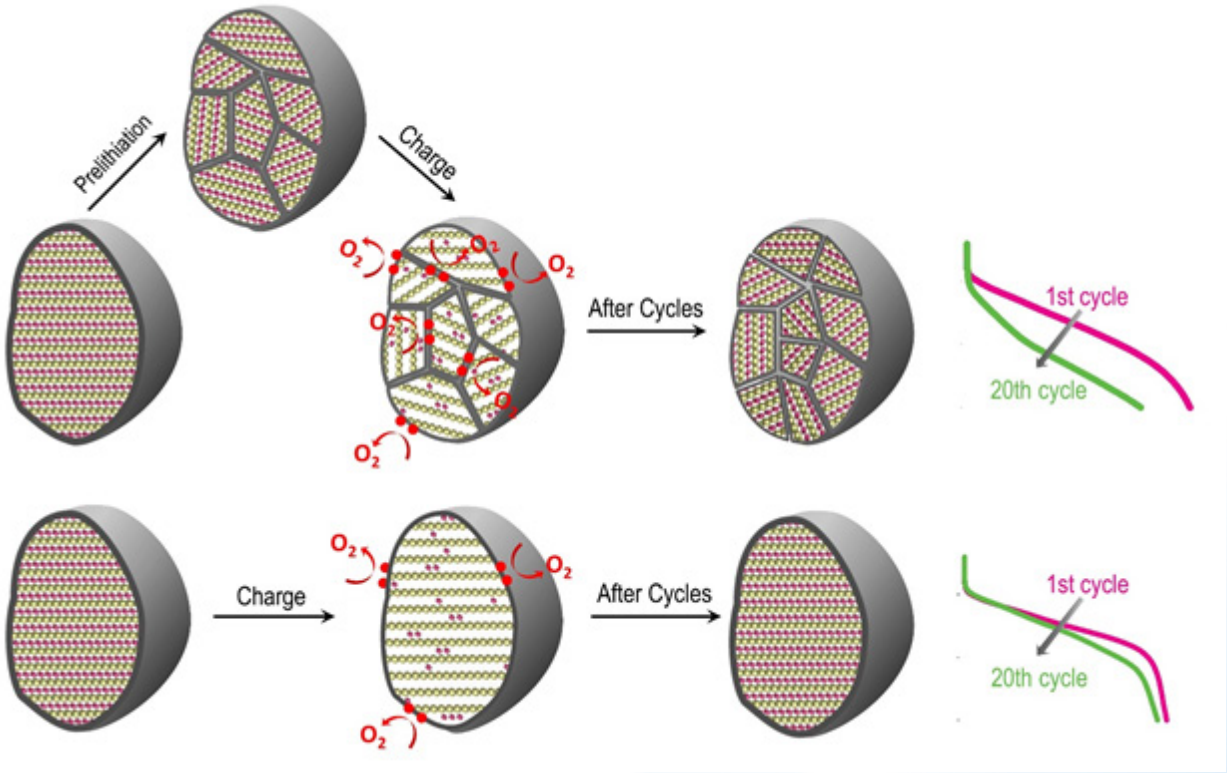
Enyuan Hu *et. al.*, Nano Letters, (September 2016)
DOI: 10.1021/acs.nanolett.6b01609

(a) a Z-contrast scanning transmission electron microscopic (STEM) images of pristine sample and "OCV—1V—3V" sample. In the "OCV—1V—3V" sample, a few selected domains are circled out by the white lines.
(b) Illustration of the microstructure change brought by prelithiation process



Enyuan Hu *et. al.*, Nano Letters, (September 2016)
DOI: 10.1021/acs.nanolett.6b01609

Illustration of prelithiation-induced smaller crystallite size and its effect on voltage fade in $Li_2Ru_{0.5}Mn_{0.5}O_3$.



Enyuan Hu *et. al.*, Nano Letters, (September 2016)
DOI: 10.1021/acs.nanolett.6b01609

Battery500 Consortium

- The Battery500 Consortium aims to triple the specific energy (to 500 WH/kg) relative to today's battery technology while achieving 1,000 electric vehicles cycles.

- The consortium aims to overcome the fundamental scientific barriers to extract the maximum capacity in electrode materials for next generation Li batteries.

- The consortium leverages advances in electrode materials and battery chemistries suppor

Pacific Northwest NATIONAL LABORATORY

STANFORD UNIVERSITY

SLAC NATIONAL ACCELERATOR LABORATORY

TESLA

THE UNIVERSITY OF TEXAS AT AUSTIN

UC San Diego

UNIVERSITY of WASHINGTON

IBM

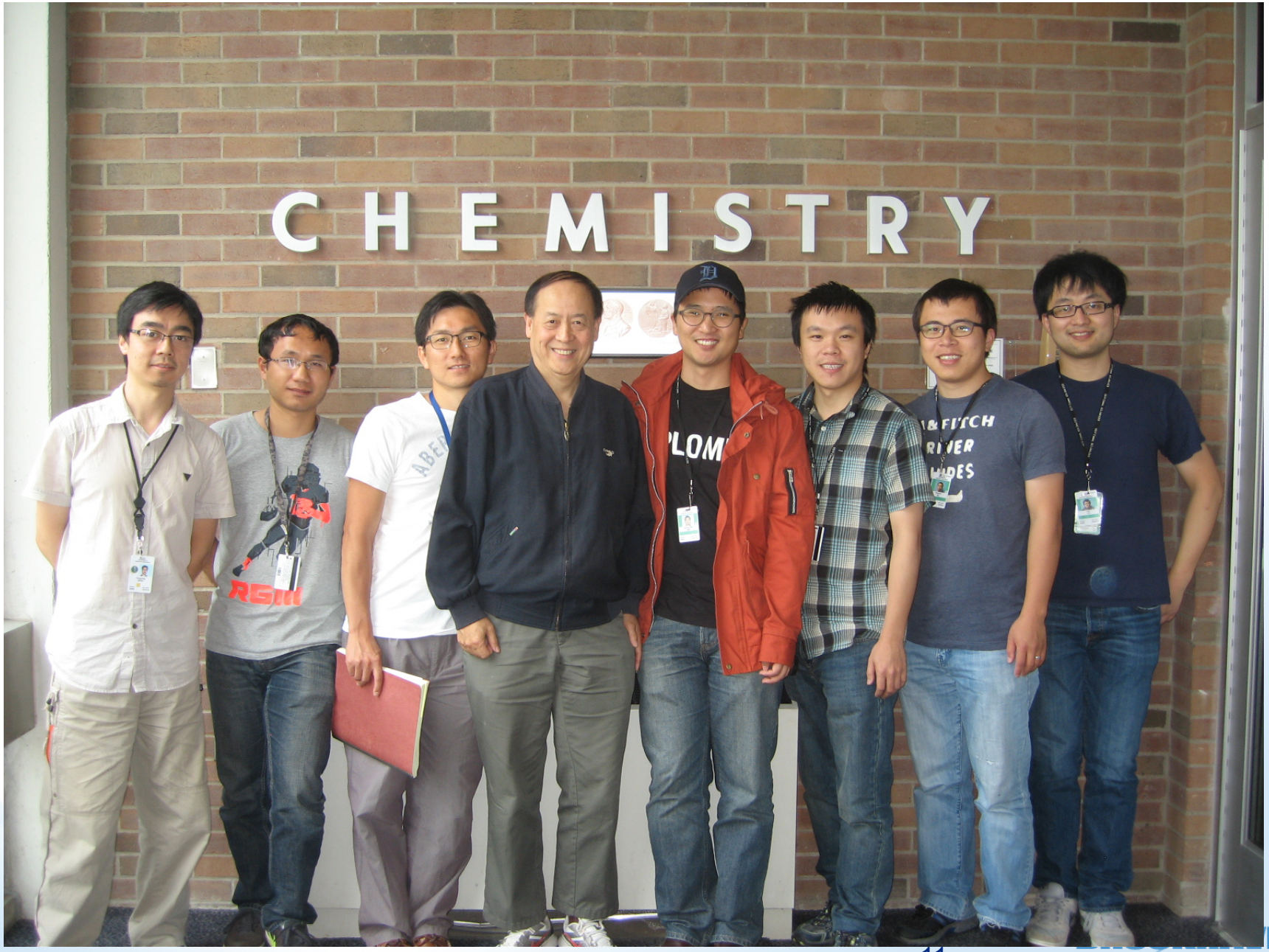
BROOKHAVEN NATIONAL LABORATORY

BINGHAMTON UNIVERSITY

INL Idaho National Laboratory

Consortium Battery500

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy


CHEMISTRY