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Advanced Na-ion battery: Towards Co-free cathodes

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DOE-OE Peer Review
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PNNL is operated by Battelle for the U.S. Department of Energy

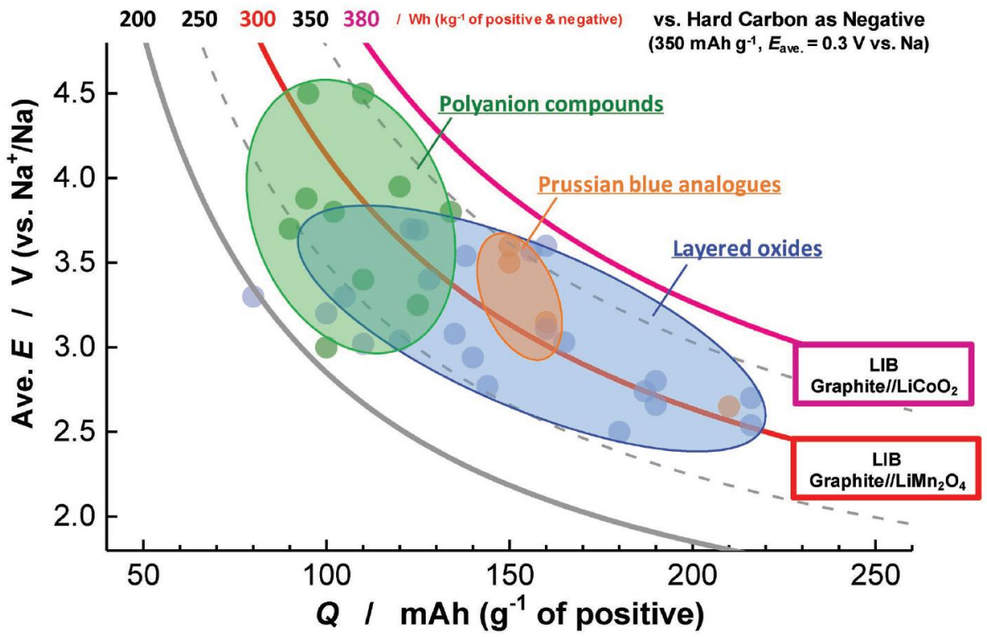
Project overview

- Low cost materials for sodium-ion batteries
- Materials scaleup and pouch cell assembly
- Mechanism study

Stationary Energy Storage

E-bikes

Electric Vehicles



S. Komaba et al., Adv. Energy Mater., 2018, 8, 17, 1703415
Statista.com, Interatec

Project objectives

- Develop Co-free layered cathode materials with reduced amount of Ni.
- Understanding of the material structure.
- Large cell performance evaluation.

Project challenges

- Replacing Co and reducing the use of Ni limit the material capacity.
- Stoichiometry and structure optimization.
- Material scale-up and synthesis condition optimization.

Project milestones in FY20

- **Milestone 1.**

Demonstration of 50 mAh Na-ion battery pouch cell with Gen 2 cathode (Ni rich NMC material) with >80% retention over 100 cycles

- **Milestone 2.**

Develop Co-free cathode material that demonstrates comparable performance with the Gen 2 material

- **Milestone 3.**

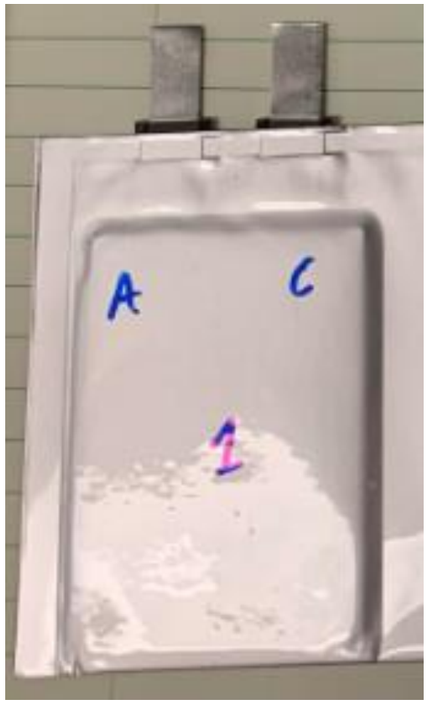
Publishing 2 high impact journal articles on advanced Na-ion battery materials

Project achievements in FY20

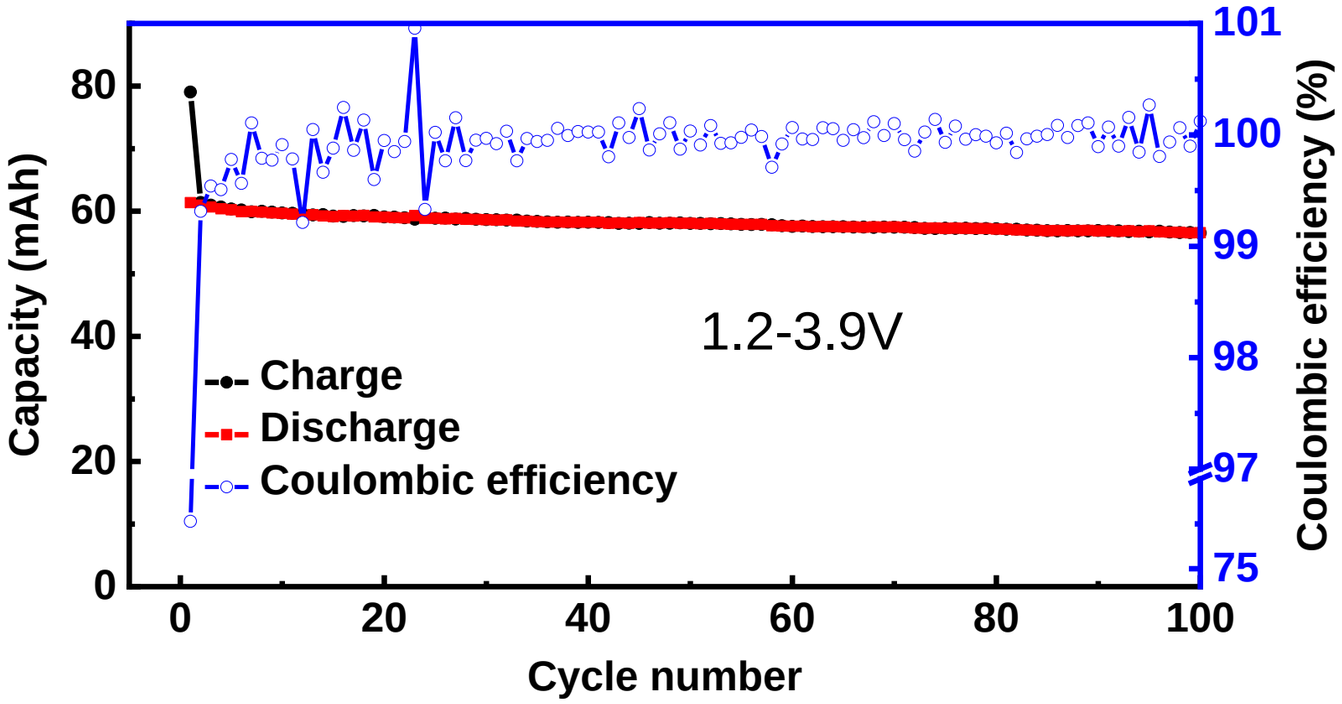
- **Research highlights**
- Gen 2 (Ni-rich NMC) synthesis was scaled up to 100 g scale per batch.
- A group of layered materials with no Co and 40% less Ni has been demonstrated, the performance reaches 130 mAh/g with 90% retention after 500 cycles.
- A new strategy to prohibit O3-P3 phase transition was demonstrated both experimentally and theoretically.
- **Publications (Two papers and one invention report in preparation)**
- F. Omenya et al., Encyclopedia of Energy Storage, Elsevier, 2020
- J. Song et al., ACS Energy Lett. 2020, 5 (6), 1718-1725
- **New collaborations established**
- Prof. Xin Li at Harvard University
- Dr. Enyuan Hu at Brookhaven National Laboratory
- **Professional activities**
- Co-organizing the ACS Spring Meeting Battery Symposium (to be held in March 2021)

Project achievements in FY20 (1)

Single layer pouch cell cycling extended from 50 times to 100 times with 91% retention.



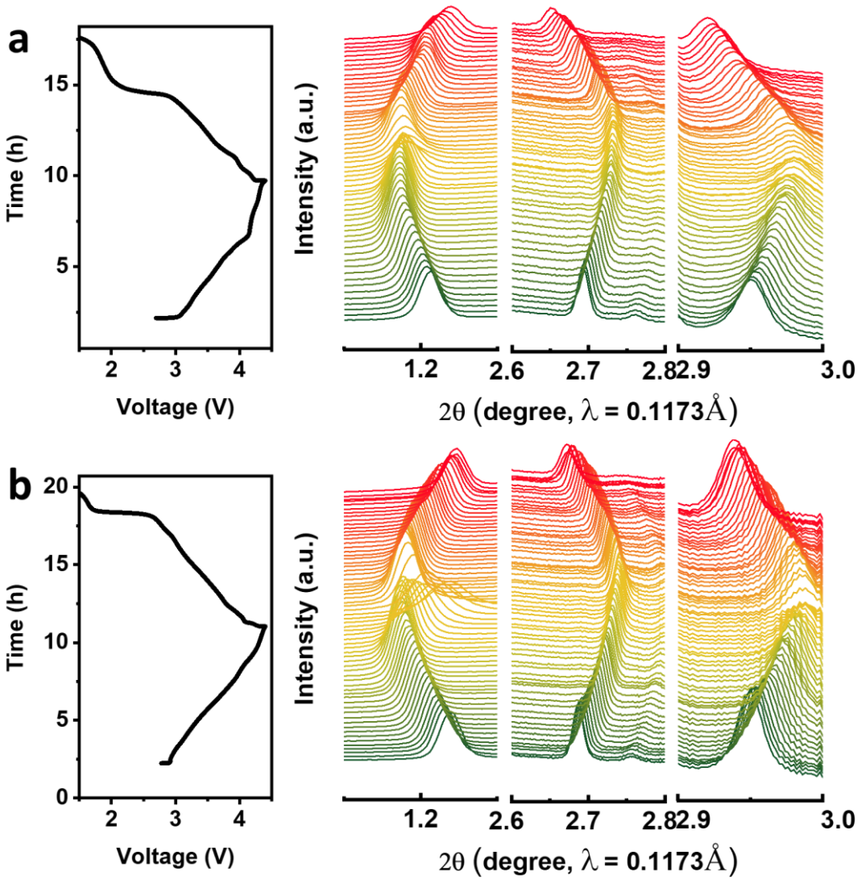
Gen 2 Ni-rich NMC: O3-$NaNi_{0.68}Mn_{0.22}Co_{0.10}O_2$



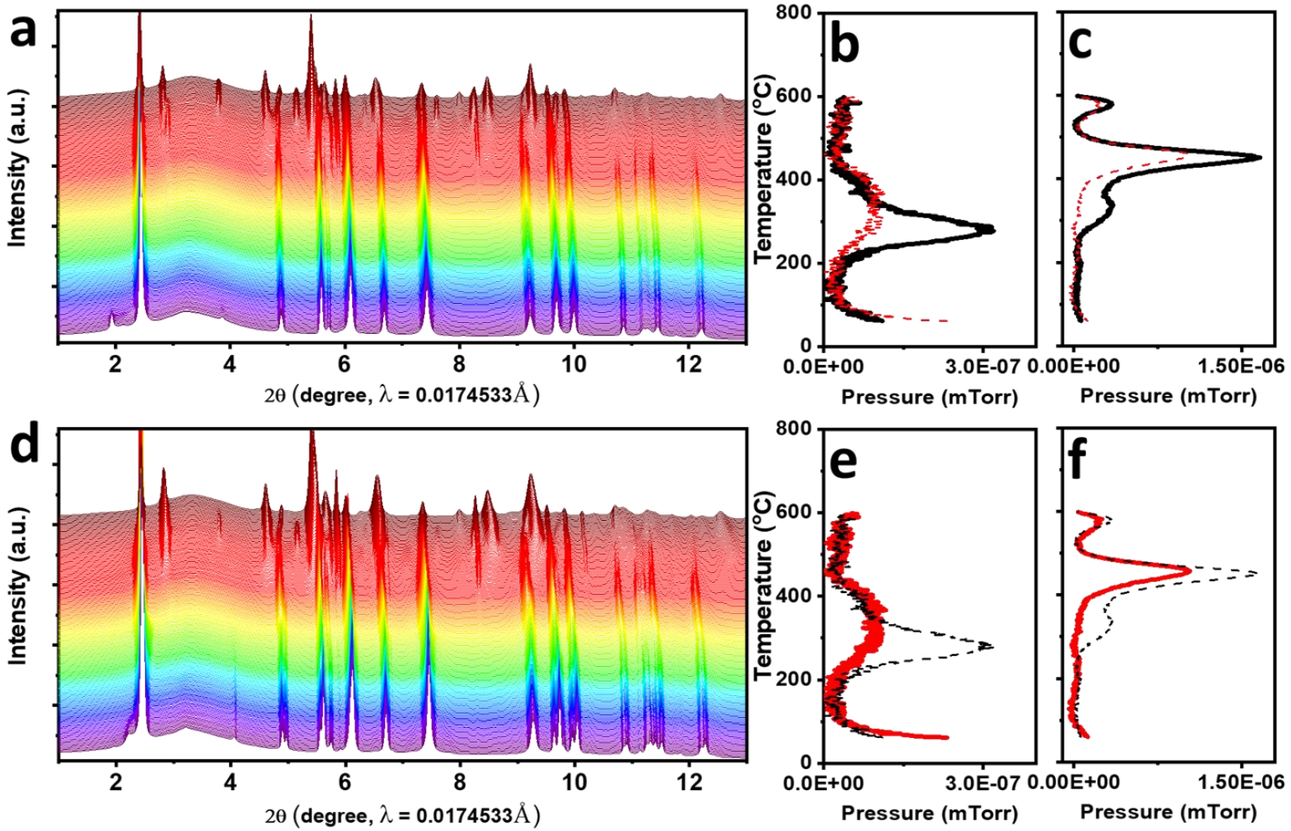
Project achievements in FY20 (2)

Structural evolution and stability measurement of P2 and Li doped P2 materials

in-situ XRD measurements during cell operation

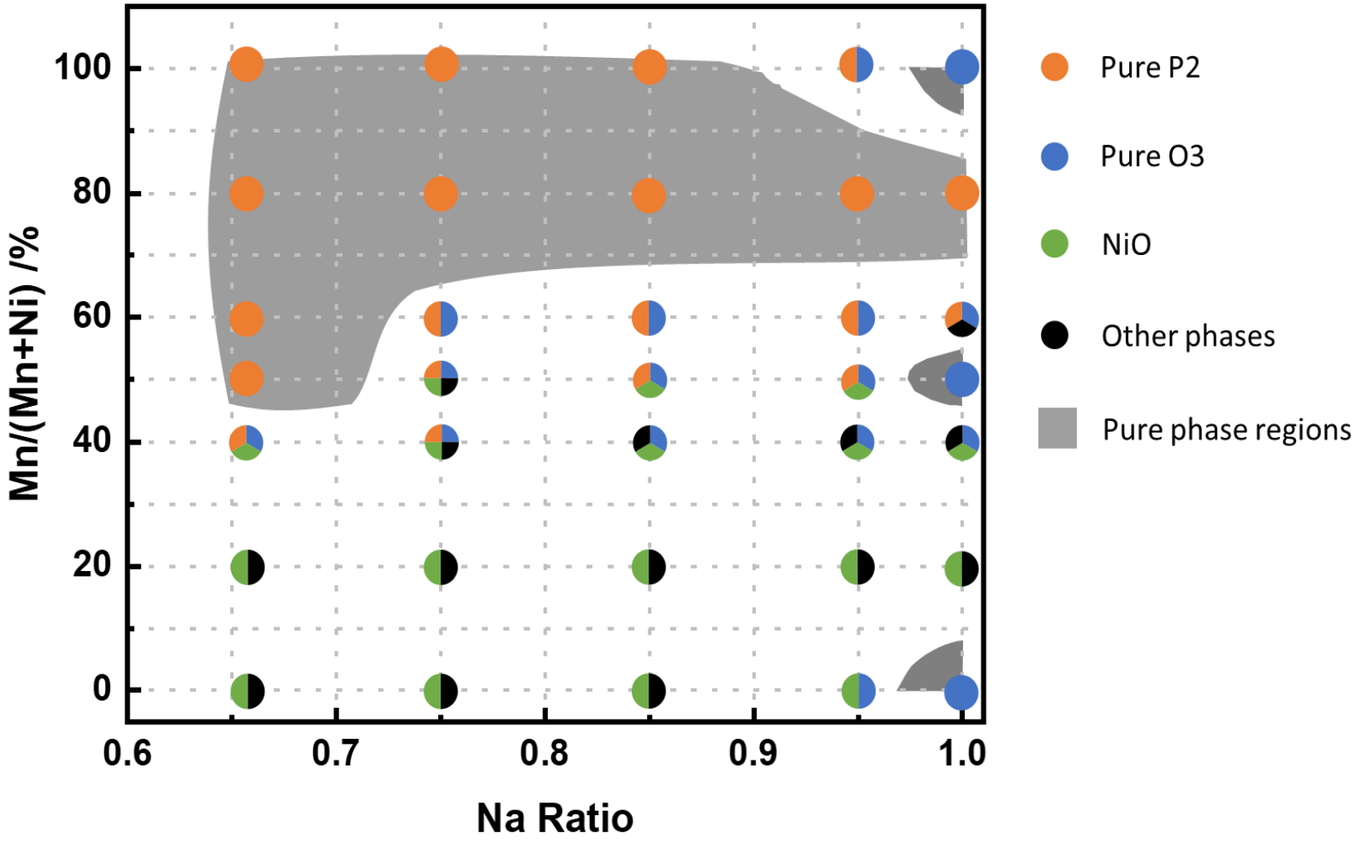


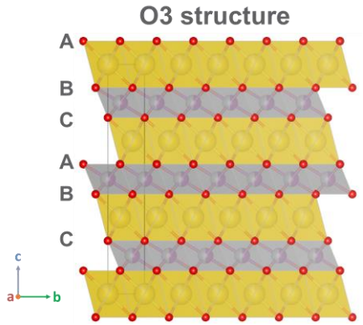
In-situ XRD during charged sample heating, mass spectroscopy of O_2 and CO_2 release during the heating process



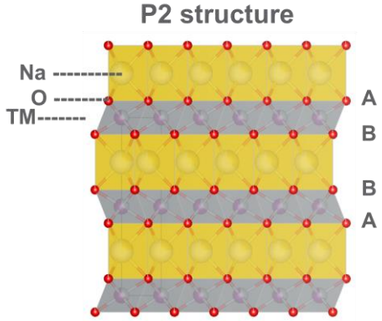
Project achievements in FY20 (3)

Phase diagram of $Na_xMn_yNi_{1-y}O_2$ – A guide to the design of P2/O3 hybrid material





Pros:
High Na stoichiometry
Cons:
Adverse phase transition
High Na diffusion barrier



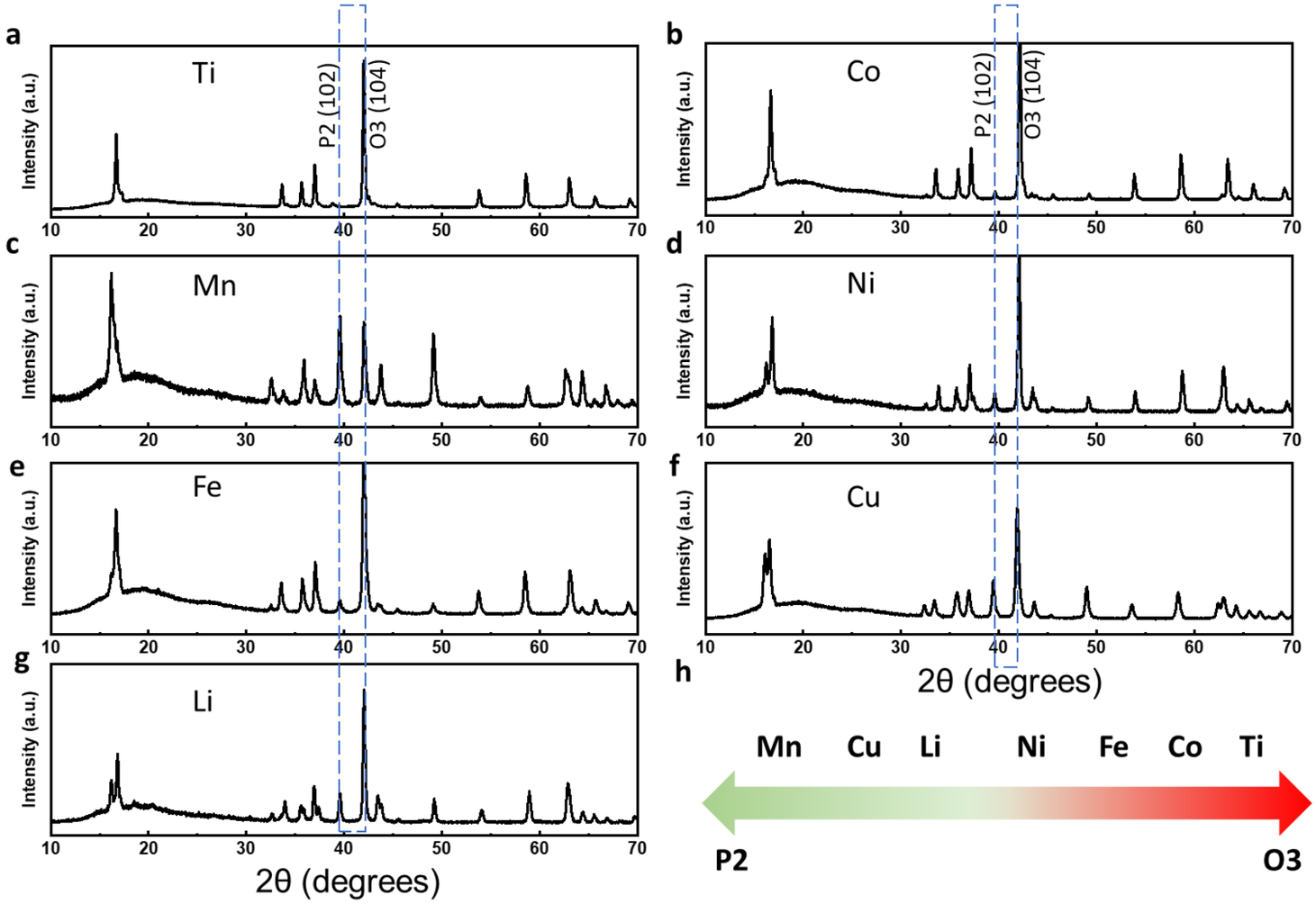
Pros:
Low Na diffusion barrier
Cons:
Adverse phase transition
Low Na stoichiometry

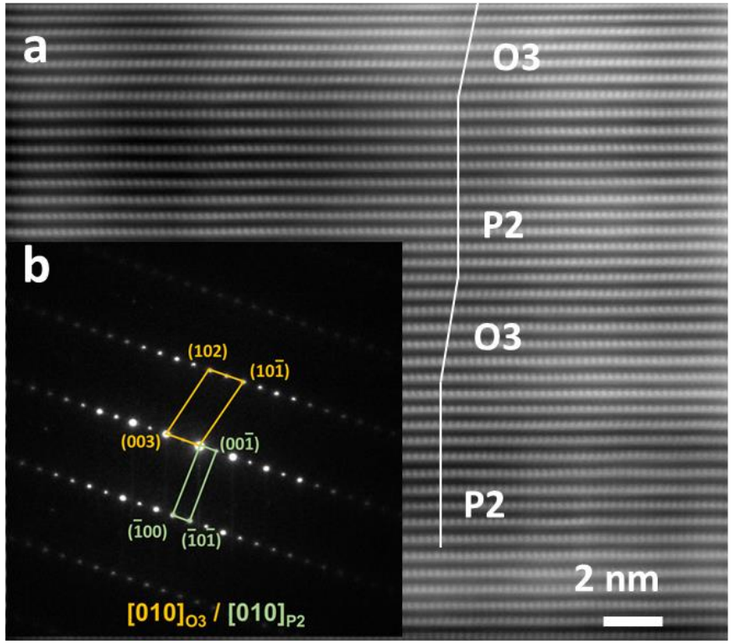
Layered cathode materials are mainly constructed based on the composition tailoring of $Na_xMn_yNi_{1-y}O_2$, but there is no summary of the phase diagram.

B. Xiao et al., in prepration

Project achievements in FY20 (3)

Phase construction with alien element doping: $Na_xMn_yNi_zM_{1-y-z}O_2$



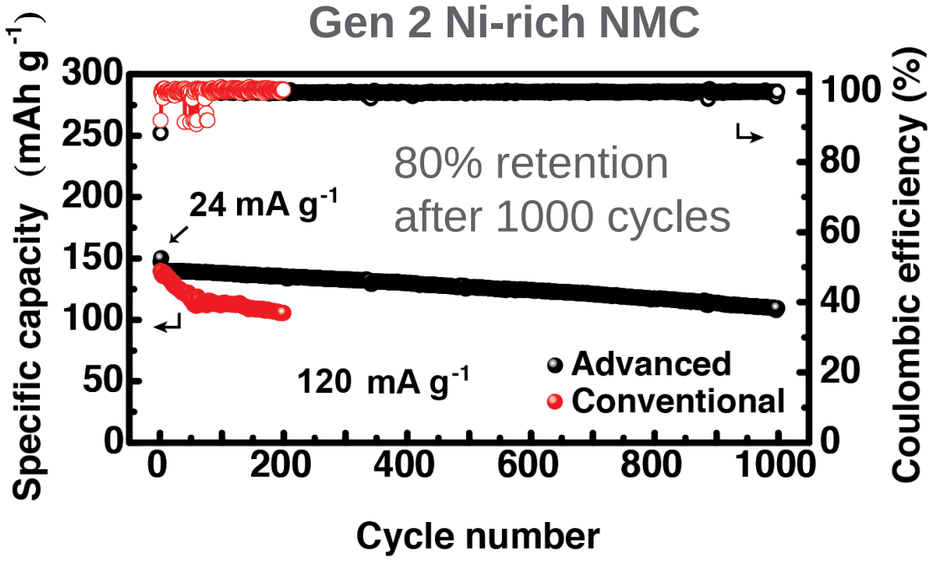


With the composition fixed to $Na_xMn_yNi_zM_{1-y-z}O_2$, it is possible to investigate the role of element M in determining the final phase and tailor the relative amount of P2 and O3 phases.

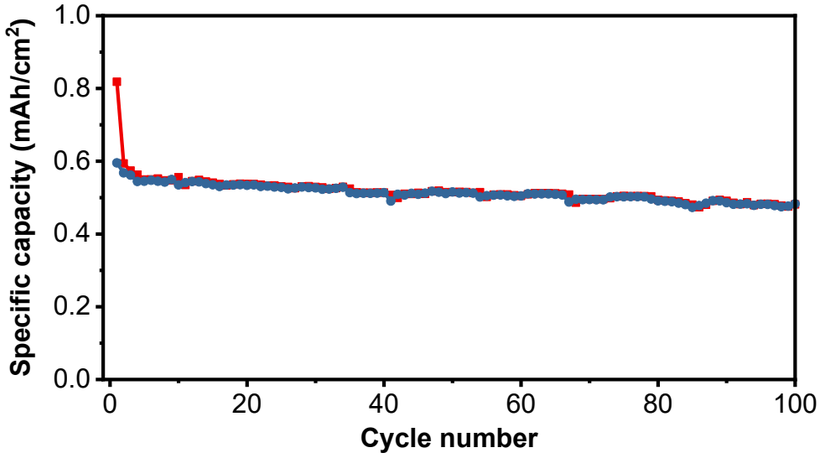
Project achievements in FY20 (3)

$Na_xMn_yNi_zM_{1-y-z}O_2$ compared with the Gen 2 Ni-rich NMC

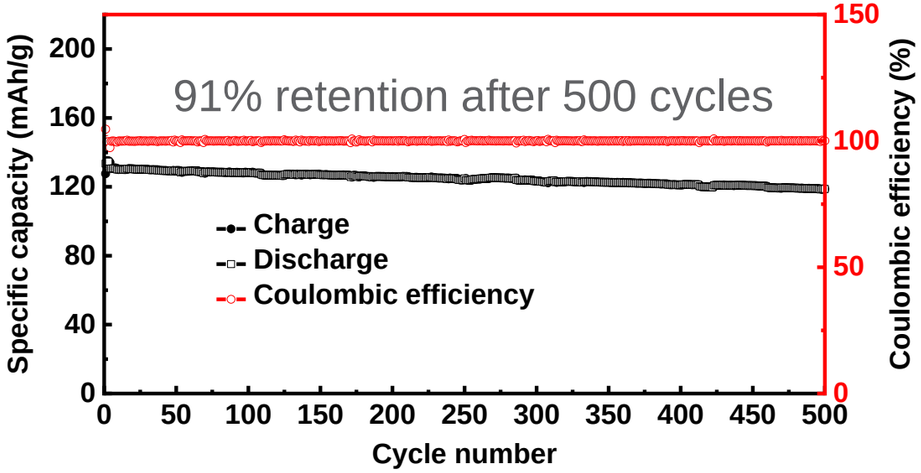
Gen 2 Ni-rich NMC

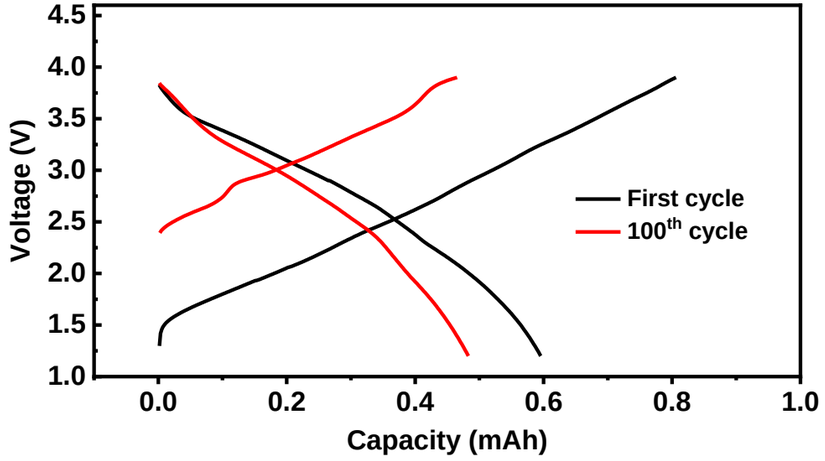


$Na_xMn_yNi_zM_{1-y-z}O_2$/hard carbon full cell



$Na_xMn_yNi_zM_{1-y-z}O_2$ *No Co, 40% less Ni*





Proposed work for FY21

- ❑ Validation of the P2/O3 hybrid materials in high loading coin cells and single layer pouch cells.
- ❑ Further reducing the amount of Ni while maintaining the capacity.

Acknowledgement and project contacts

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Thank you!

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