CREB 2025 Spring Meeting: Jun. 6, 2025

Rational Design of Battery Cathode Materials to Battery Cell Prototyping at BEACONS

BEACONS

BATTERIES and ENERGY to ADVANCE COMMERCIALIZATION and NATIONAL SECURITY

KJ Cho

Energy Storage Systems Campus funded by DoD

BEACONS center

https://beaconsusa.org/

Department of Materials Science and Engineering,
The University of Texas at Dallas
Richardson, Texas 75080, USA

LEAP MANUFACTURING

THE UNIVERSITY OF TEXAS AT DALLAS

BEACONS
(Batteries and Energy to Advance COmmercialization and National Security)

Support

Manufacturing Capability Expansion and Investment Prioritization office within the Department of Defense.

Associated the DOD Scaling Capacity and Accelerating Local Enterprises (SCALE) program, an initiative to create sustainable technologies that support our national security efforts.

Mission

To advance the commercialization and security of the nation's energy storage systems by developing a resilient and sustainable domestic supply chain through transformative technology, agile infrastructure, and an accomplished workforce.

UTD Battery Initiative: 2022 fall (UTD President Benson)

→ BEACONS Center (Sep. 2023)

ML/AI design of battery materials

High throughput robotic synthesis of battery materials

Diverse funding sources

DoD funded BEACONS Center

R&D line of LIB cells

Next-gen solid state batteries

Aqueous Zn ion batteries

Na ion batteries

Autonomous Battery Cell (ABC) Lab: Samsung AML collaboration (Sep. 2022)

KJ Cho

Yue Zhou

Cormac Toher

Shuang Cui

Guoping Xiong

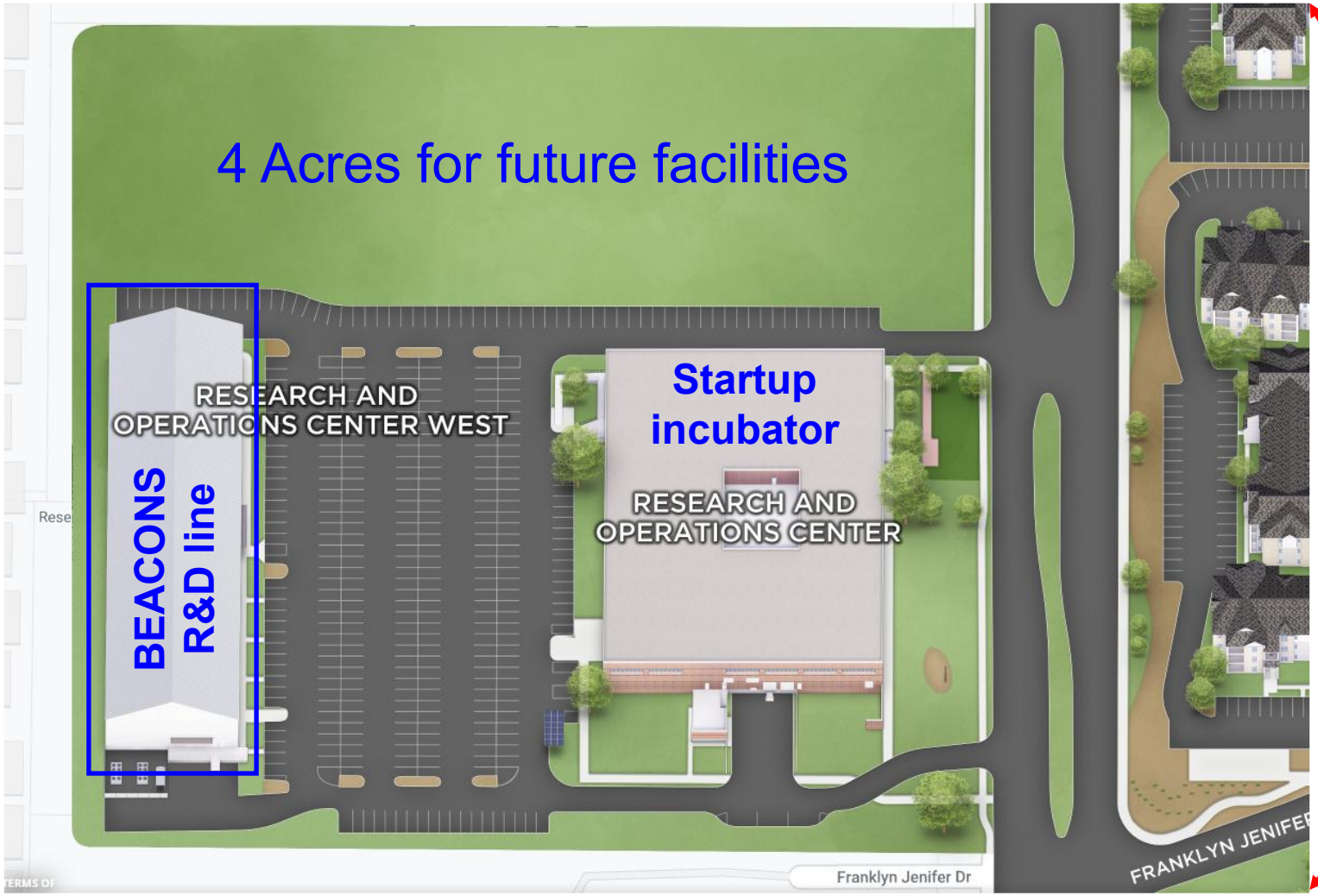
Mihaela Stefan

Laisuo Su

Shirley Meng (U Chicago, ANL)

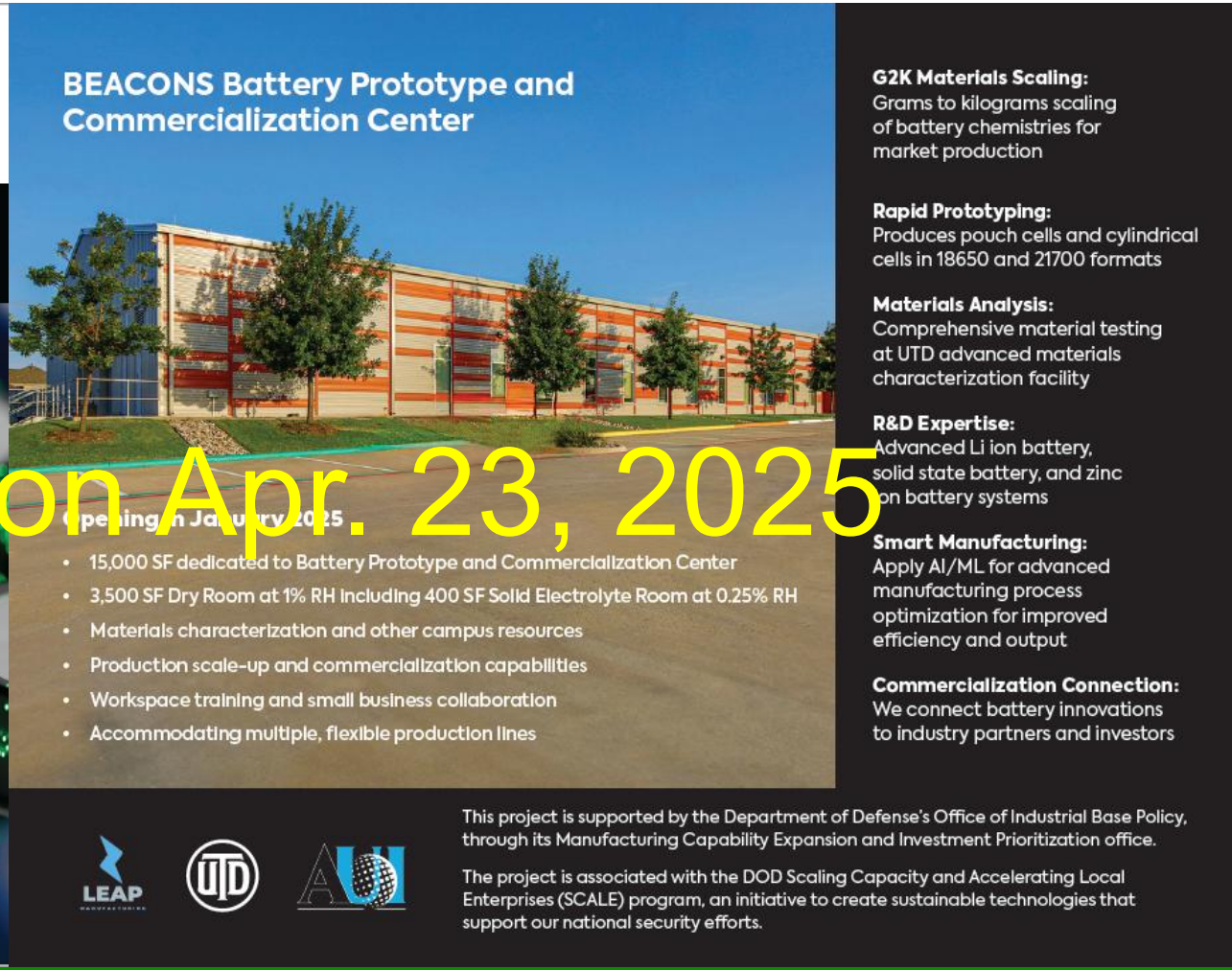
Kristin Persson (UC Berkeley, LBNL)

BEACONS Battery R&D Line at ROC West



BEACONS center summary

BEACONS Center to bridge battery research to battery manufacturing.



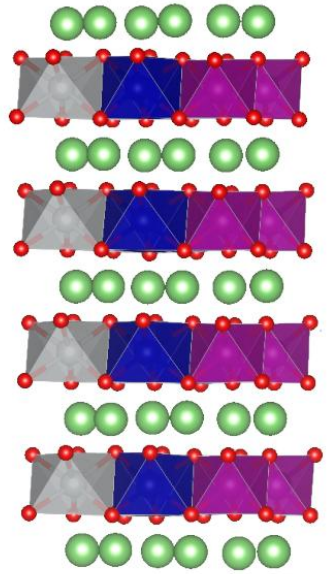
Opening event on Apr. 23, 2025

Rational Design of Battery Cathode Materials

LIB cathodes: ~50% of LIB cell cost
LIB cell energy density ≅ ~1/3 of cathode energy density
LCO: 150 Ah/kg × 3.7 V = 555 Wh/kg → ~200 Wh/kg cell
LNO: 230 Ah/kg × 3.7 V = 851 Wh/kg → ~300 Wh/kg cell

High-capacity Ni-rich cathode materials:
$Li(Ni,Co,Mn)O_2$ with increasing Ni

$LiCoO_2$ (LCO) → NCM111 → NCM523 → NCM622 → NCM721 → NCM811 → NCM90505 → **$LiNiO_2$ (LNO)**



$LiNiCoMnO_2$

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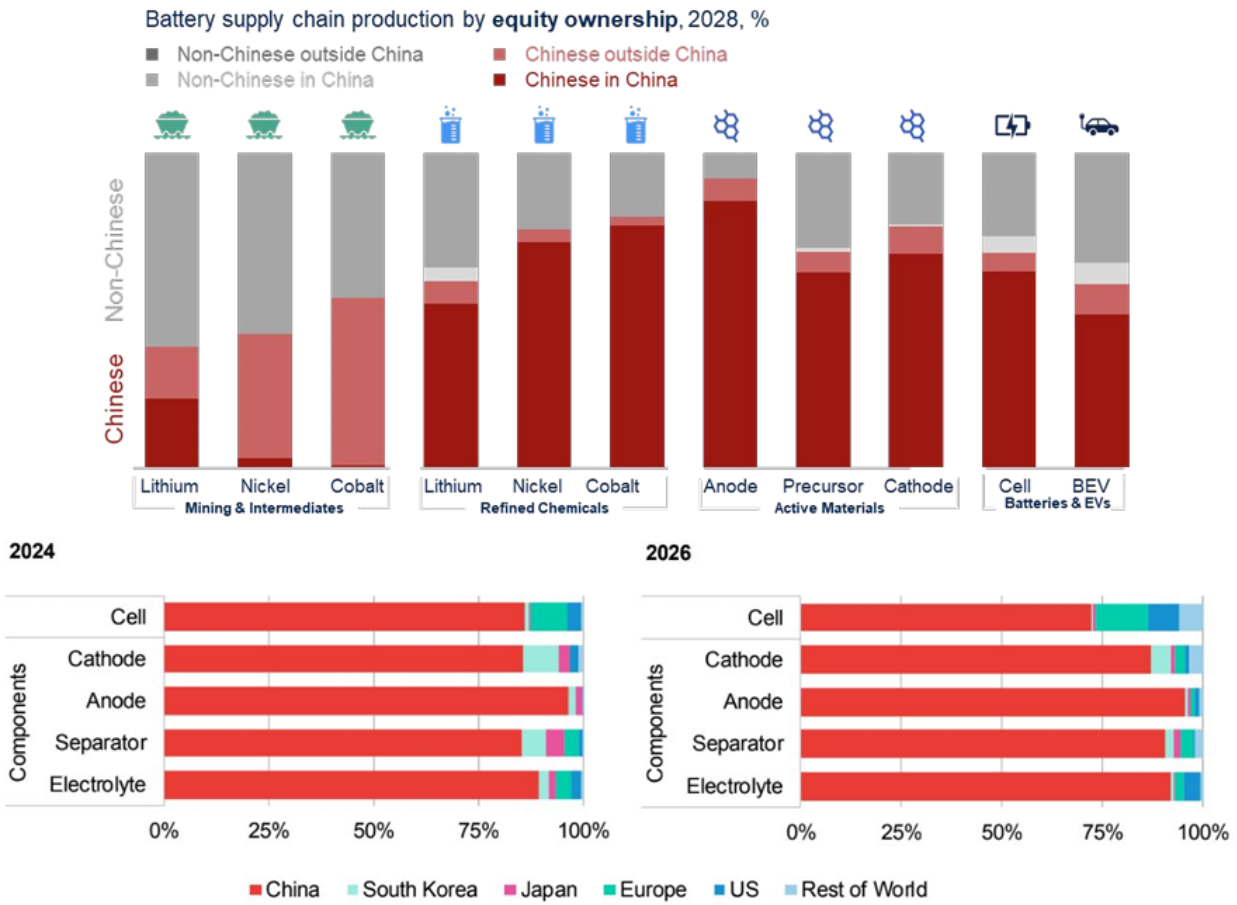
China's Ownership Of The Supply Chain Extends Beyond Its Borders

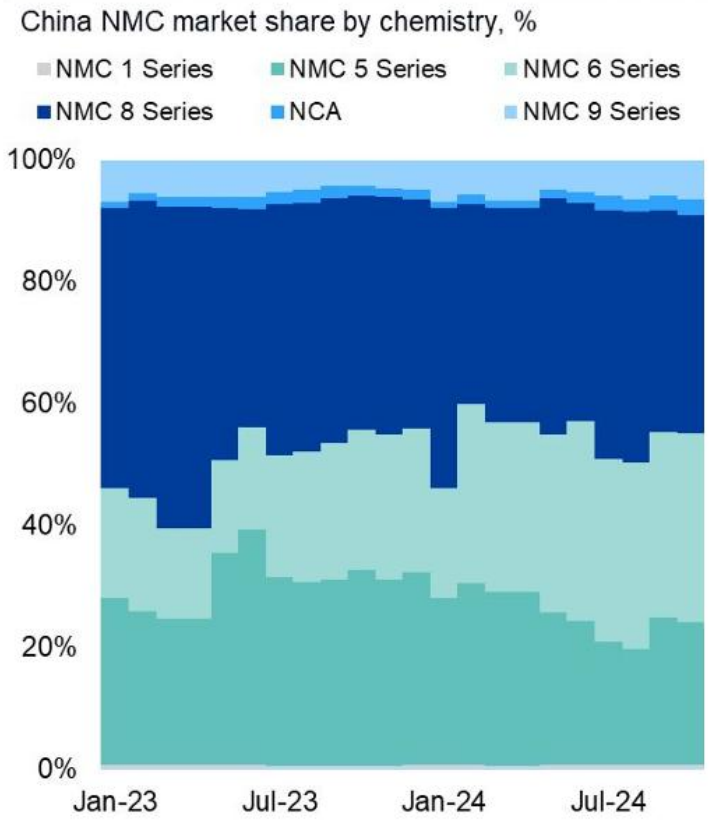


- China does not have significant geological deposits of battery raw materials, but companies have invested in overseas operations and in processing capacity at home
- This is manifested as dominance in the midstream for chemical intermediates and active materials
- Vertical integration is a strategic benefit as well as a **cost advantage**
- Despite **US FEOC rules** prompting some operations to reduce their Chinese ownership stake, many non-Chinese upstream and midstream projects have been curtailed in 2024, leaving the overall picture unchanged
- China's supply chain dominance has led to intensely competitive conditions that are squeezing non-Chinese producers

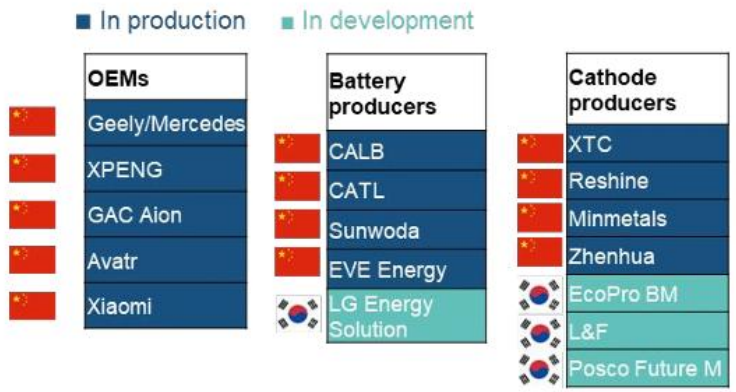
CRU BloombergNEF Source: Content & analysis provided courtesy of CRU Group (Distinguished Partner), BloombergNEF (Distinguished Partner) ; Top chart shows production by ownership; bottom charts show capacity by location.

Medium-Nickel High-Voltage Technology Is Aimed At Enhancing Competitiveness of NMC

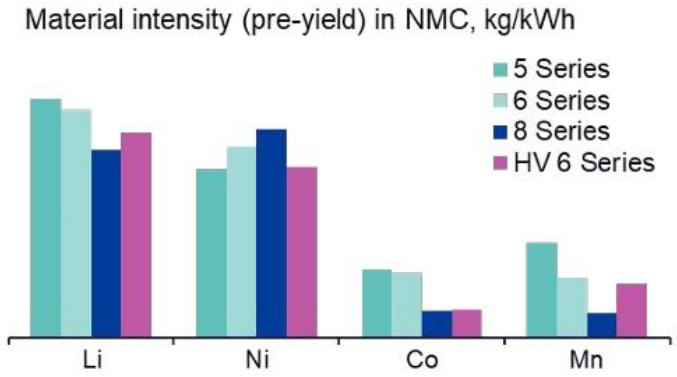
MID-Ni NOW MOST OF CHINA Ni-CATHODE MARKET



MANUFACTURER PLANS FOR MID-Ni HV CATHODE



MATERIAL INTENSITY IS ON PAR WITH NMC 811



- MNHV cathode offers the energy density of NMC 811 with the low cost of NMC 5/6 Series
- Enabled by single-crystal material
- There is a higher risk of battery degradation, but this is being mitigated
- Developed at a time of high Ni/Co prices and now increasingly adopted in best-selling BEVs
- High-voltage chemistries dampen the demand for expensive raw materials
- Several automakers are now moving back away from high-nickel chemistries

Source: Content & analysis provided courtesy of CRU Group (Distinguished Partner). For more information, visit https://www.crugroup.com. Modelled intensity for MNHV is based on NMC 631 variant

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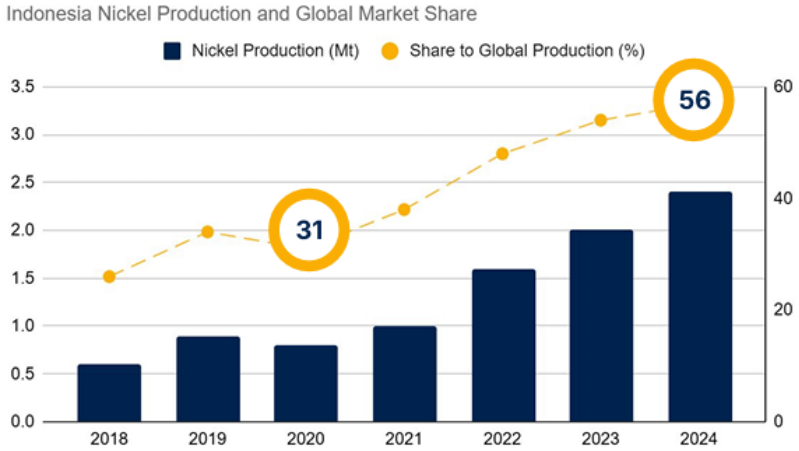
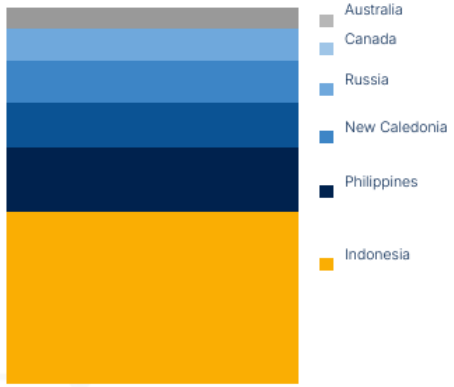
Indonesia Is Consolidating Its Dominance In The Nickel Industry

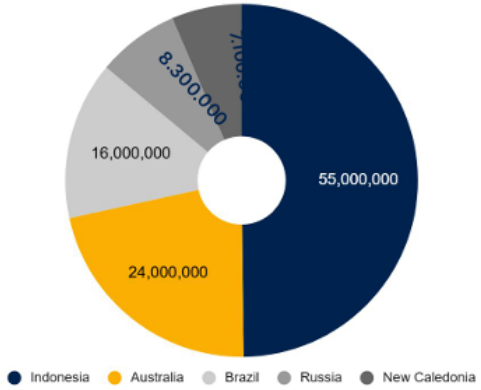
Indonesia Ni exports have increased from $4B to $35B



TOP NICKEL PRODUCERS 2024



NICKEL RESERVES (Millions mt)



NICKEL CURTAILMENT POLICY

44 smelters are currently in operation and 26 are still under construction. This condition pushes down Nickel prices in 2024 as low-cost supply floods the market.
To mitigate the oversupply condition and risks that could undermine investments and the country's lead in the market, Indonesia has:

- Imposed a moratorium on RKEF Nickel Pig Iron smelters
- Considered removing the tax holiday for RKEF smelters
- Considered a future policy that favors higher-grade nickel smelters (HPAL, which is relevant for the battery industry)

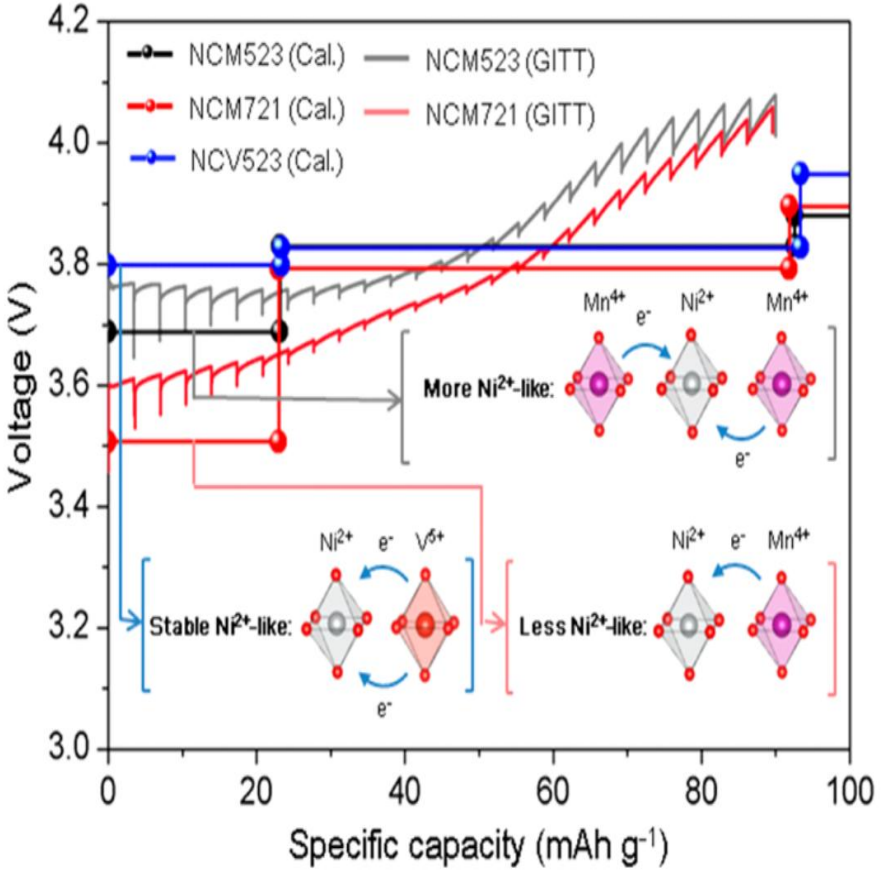
Nickel ore production in 2024 also had bureaucratic delays, resulting in massive imports from the Philippines.

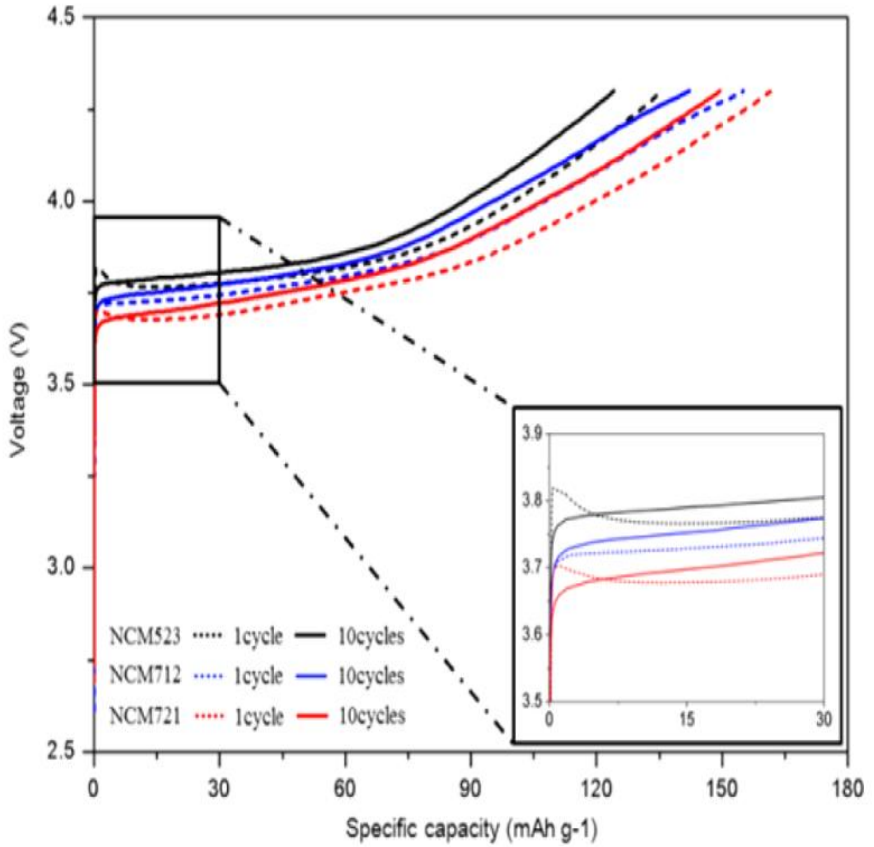
ESG COMPLIANCE

Indonesia is working to design ESG frameworks tailored to its local conditions, balancing sustainable nickel production with global market demands, and environmental responsibilities.

Source: S&P Global, SMM

Layered oxide cathodes: theory vs. experiment





D Kim, KJ Cho*, et al, Chem. Mater. 2015, 27, 6450−6456

Origin of thermodynamic instability in Ni-rich NCM materials

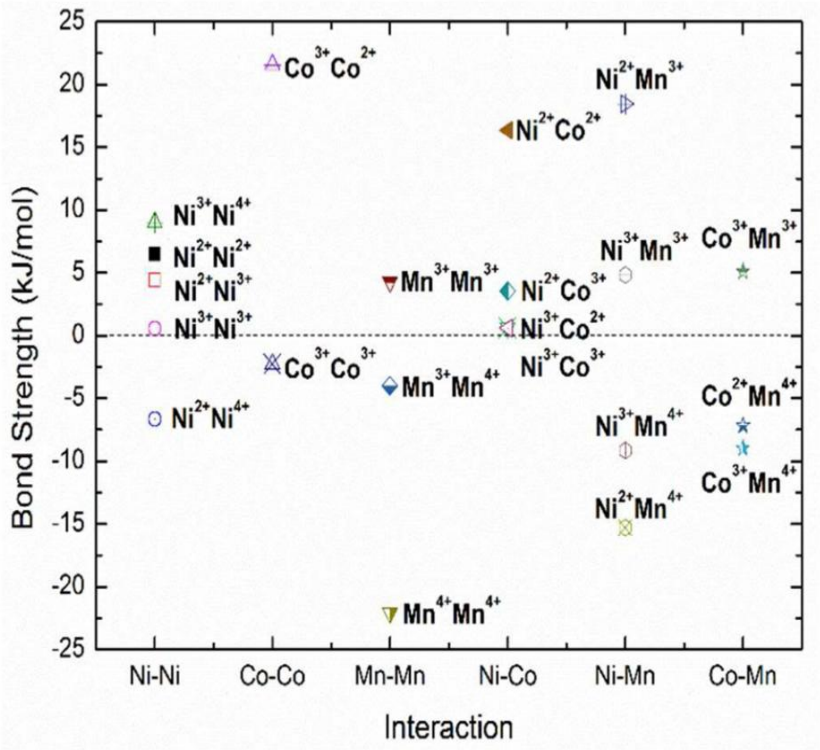


Figure 5. Bond strength for various transition metal bonds in terms of mixing energy. A negative energy means stronger bonding, and vice versa.

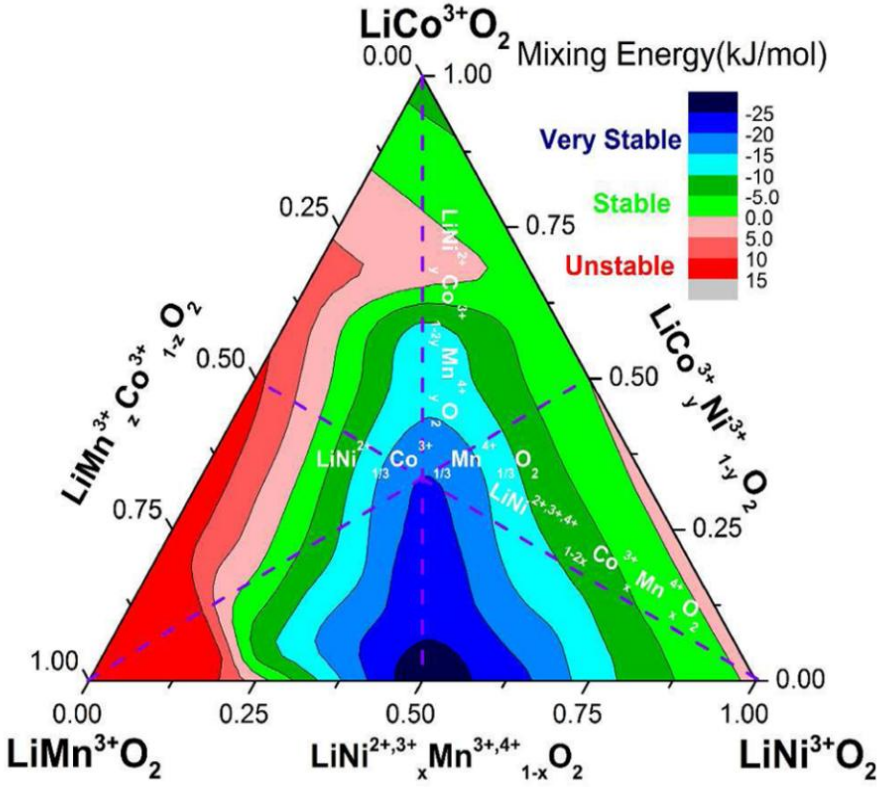
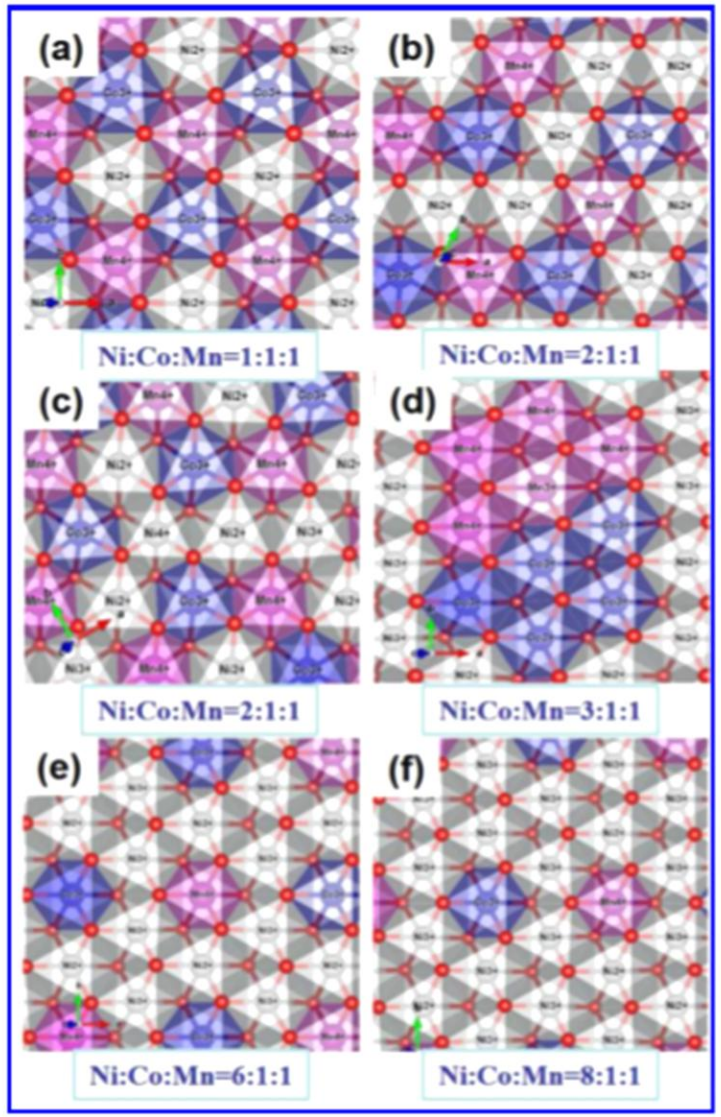
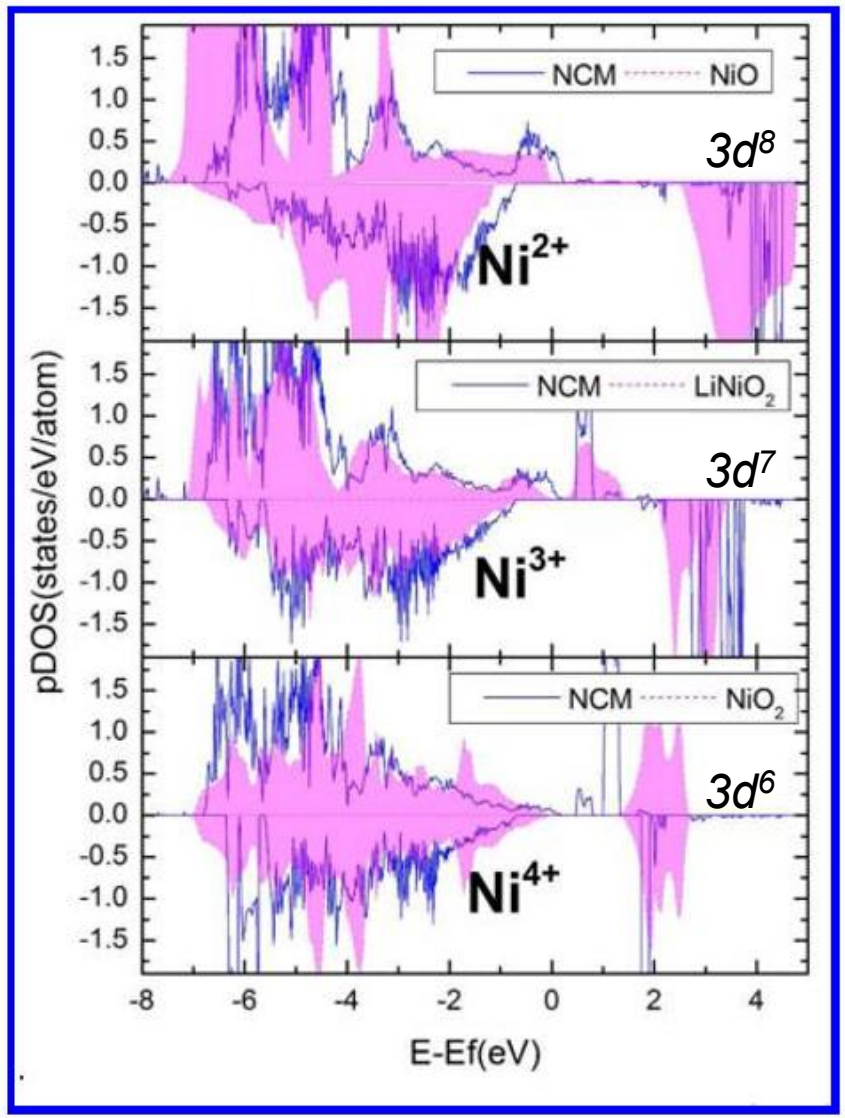


Figure 6. Mixing energy predicted from present bonding model for the solid solution $LiTMO_2$ (TM = Ni, Co, Mn) phase triangle.

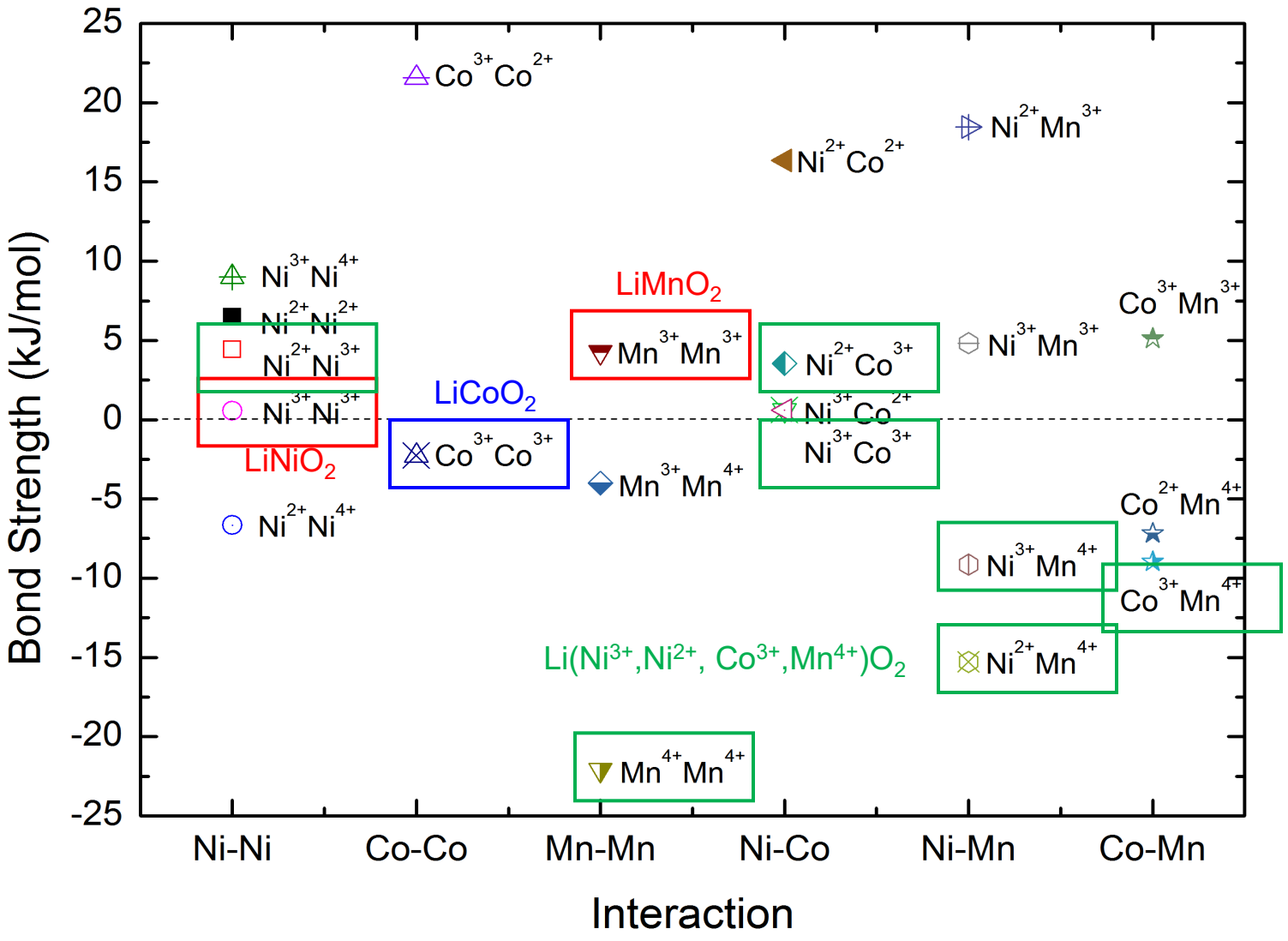
C Liang, KJ Cho*, et al, J. Phys. Chem. C 2016, 120, 6383−6393

Metal distribution in $LiNi_{1-x-y}Co_xMn_yO_2$

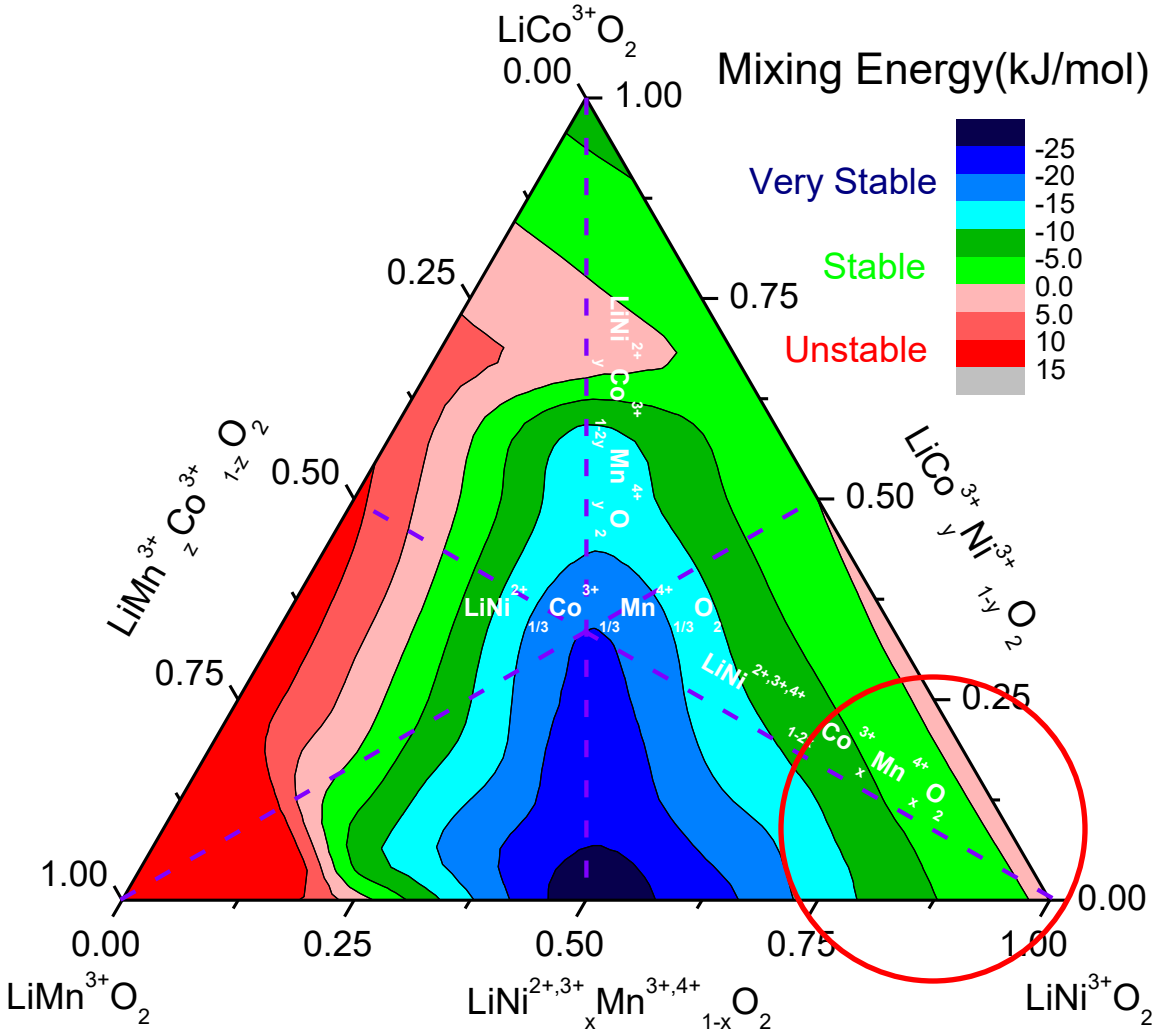




M-M effective interactions in NCM



NCM stability map



(Co, Mn)-Ni mixing in Ni-rich NCM

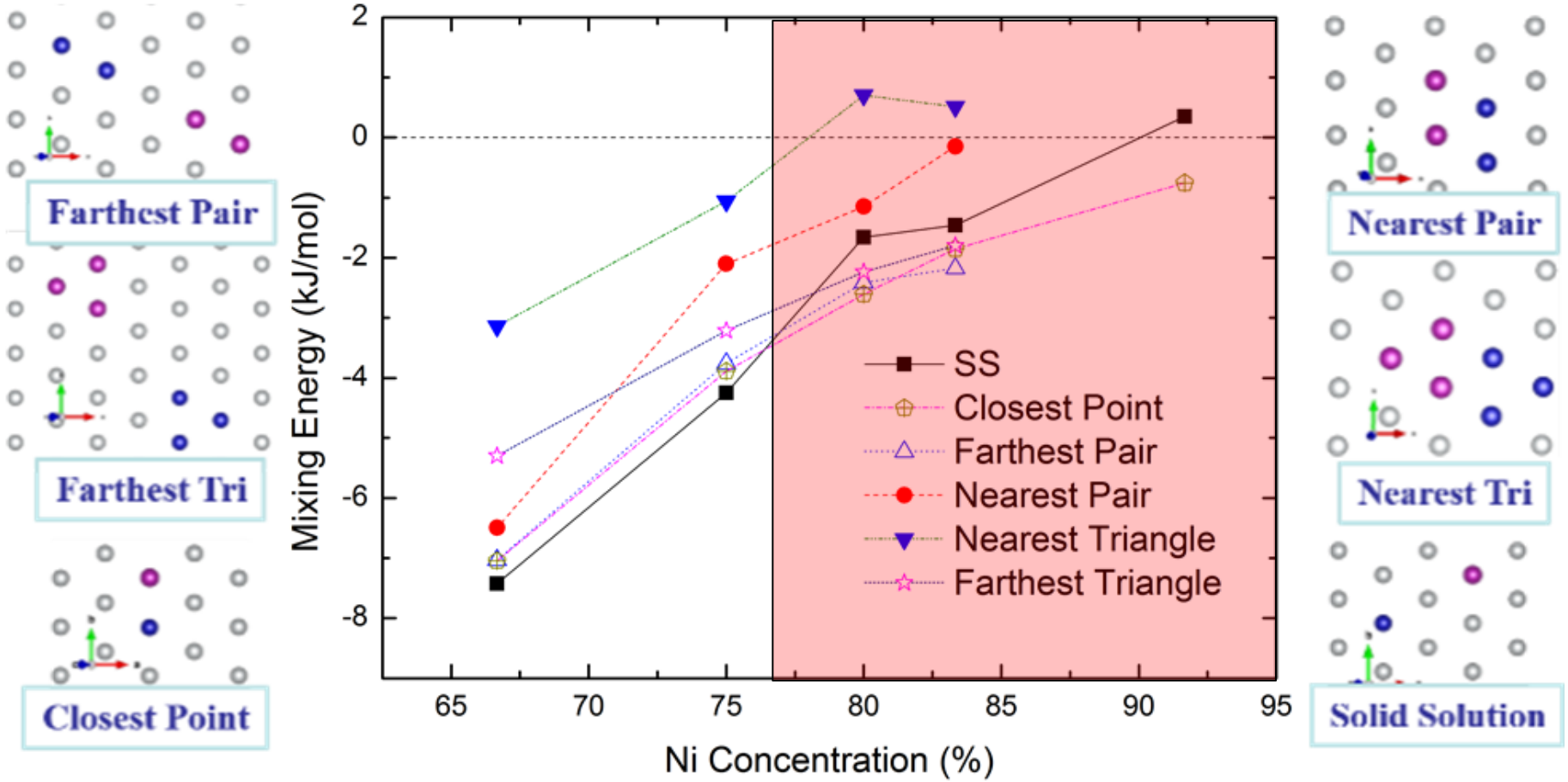
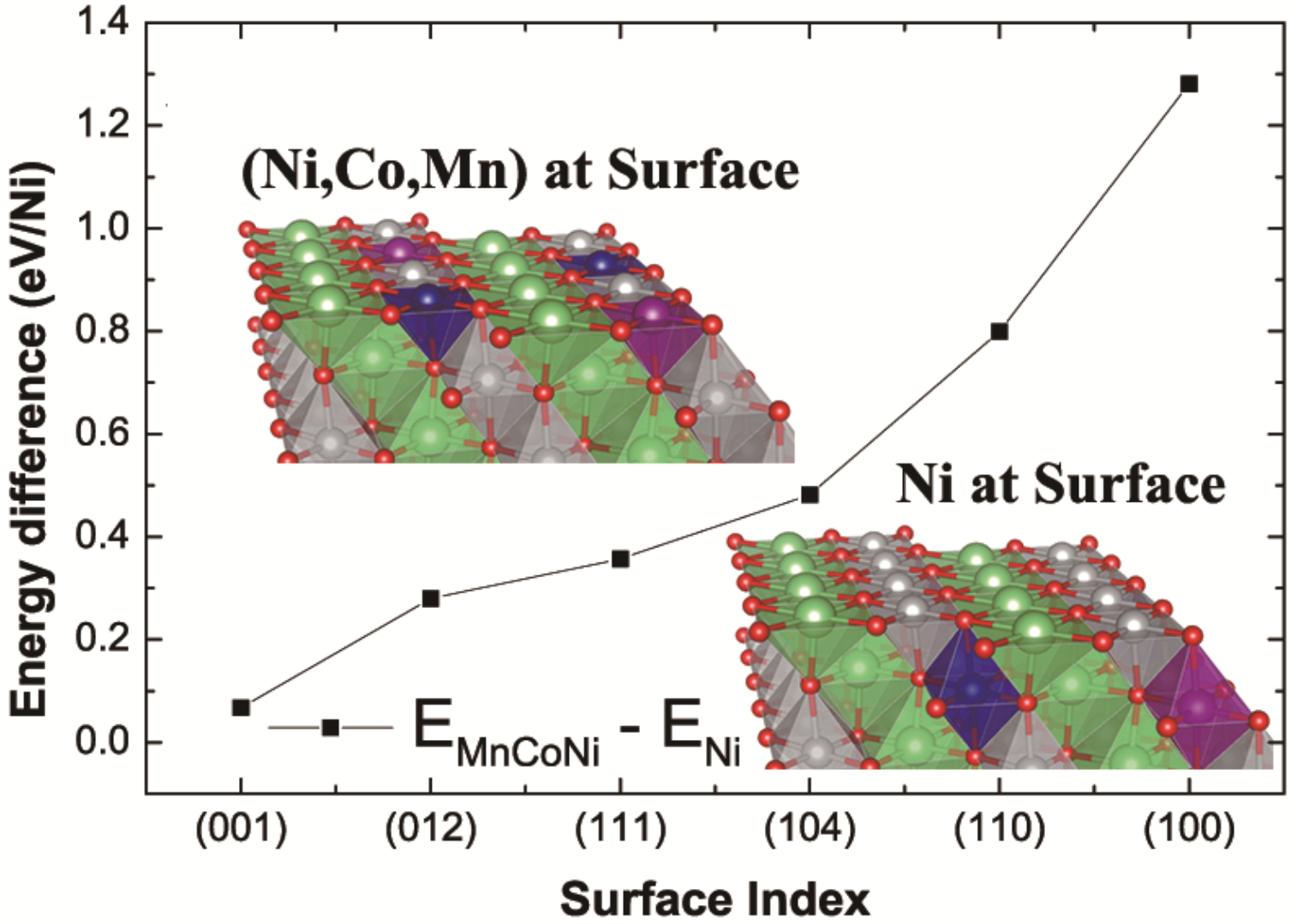
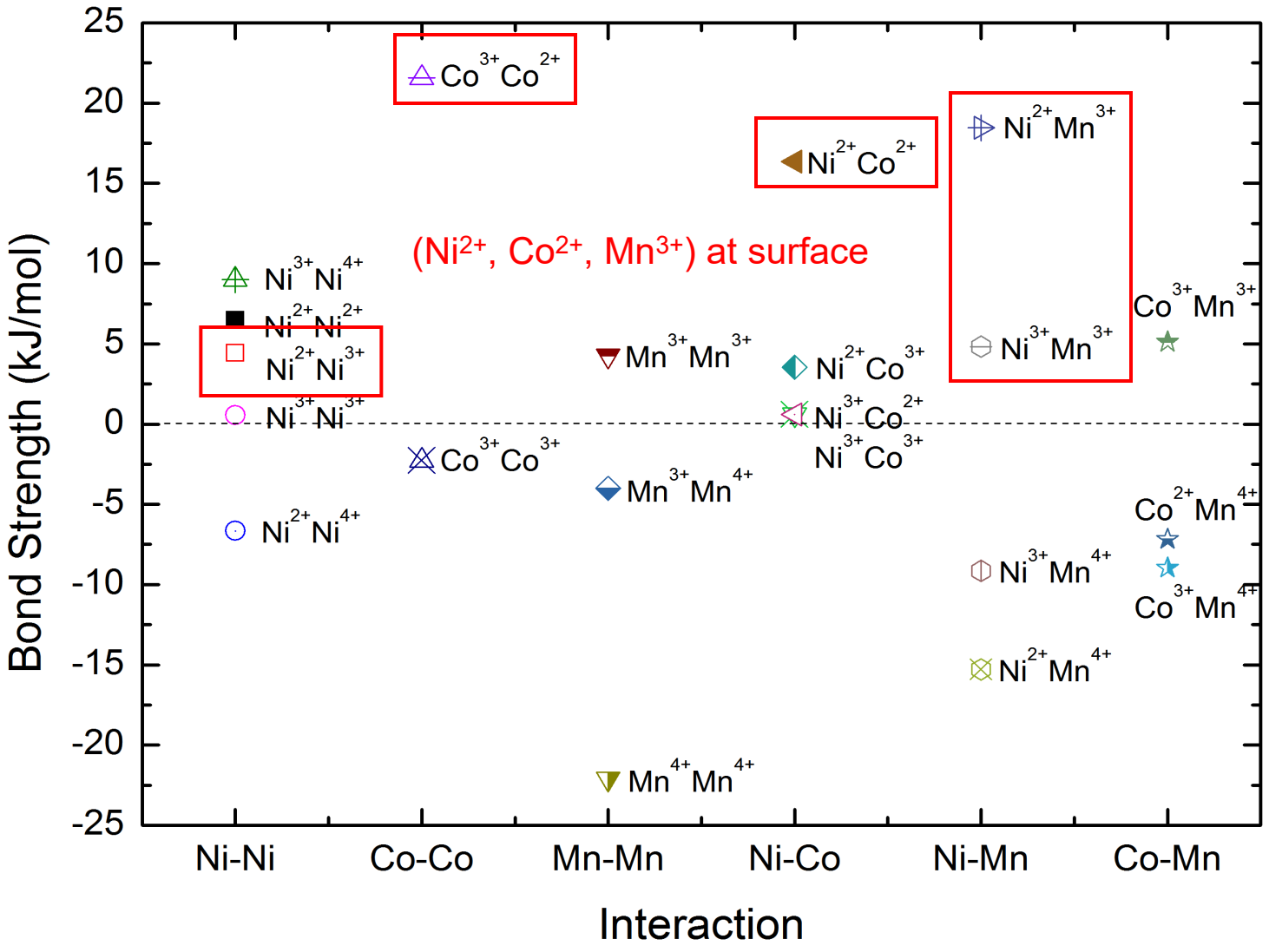


Figure 7. The mixing energies of solid solution and various cluster structures.

Ni-rich NCM811 surface: reduced metal atoms (Ni^{2+}, Co^{2+}, Mn^{3+}) at surface



M-M effective interactions in NCM



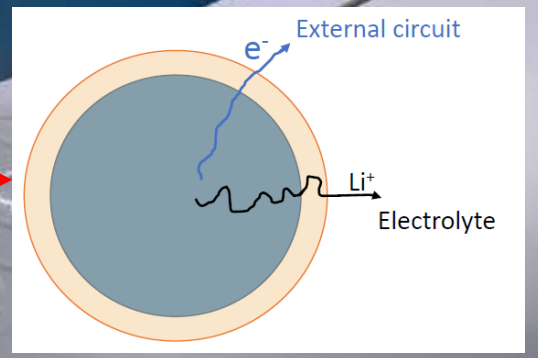
ADVANCED ENERGY MATERIALS

Full Paper

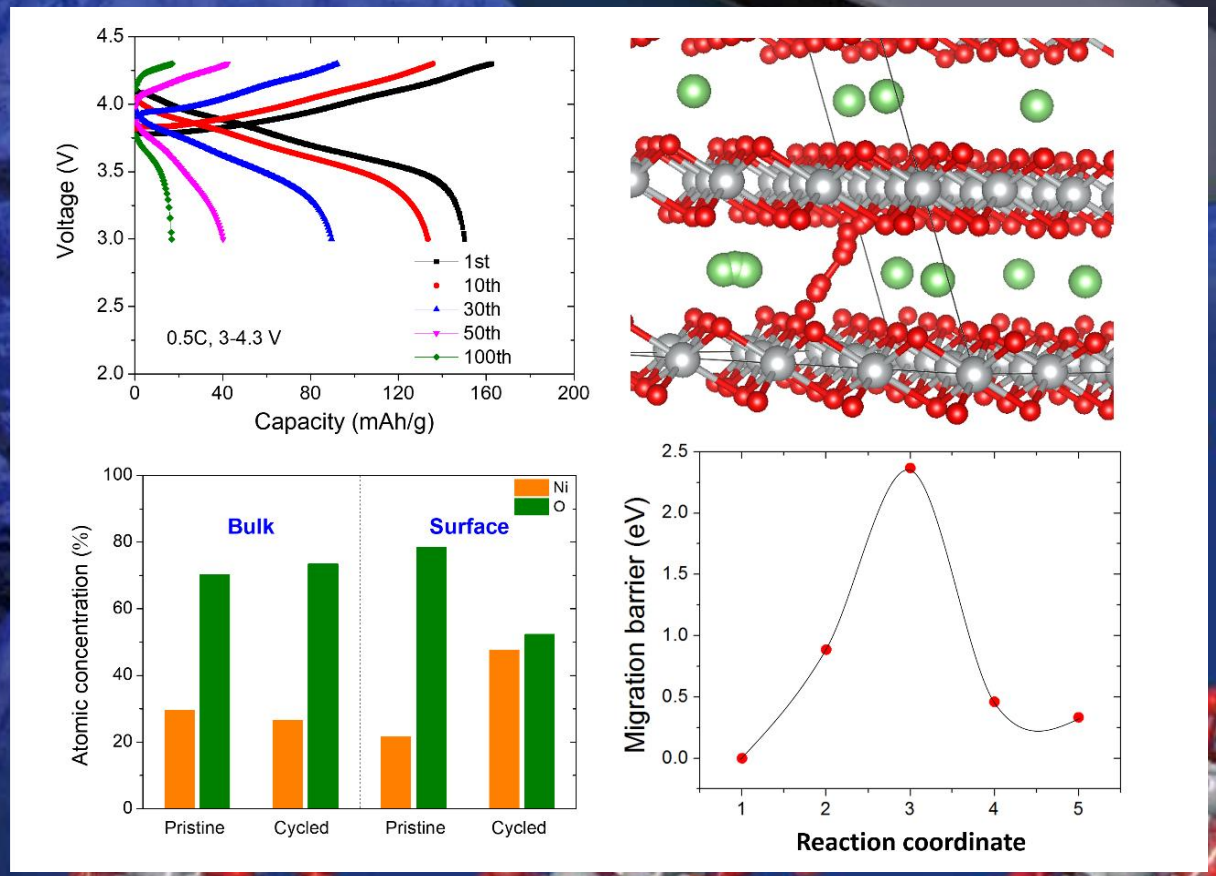
Kinetic Stability of Bulk $LiNiO_2$ and Surface Degradation by Oxygen Evolution in $LiNiO_2$-Based Cathode Materials

Fantai Kong, Chaoping Liang, Luhua Wang, Yongping Zheng, Sahila Perananthan, Roberto C. Longo, John P. Ferraris, Moon Kim, Kyeongjae Cho

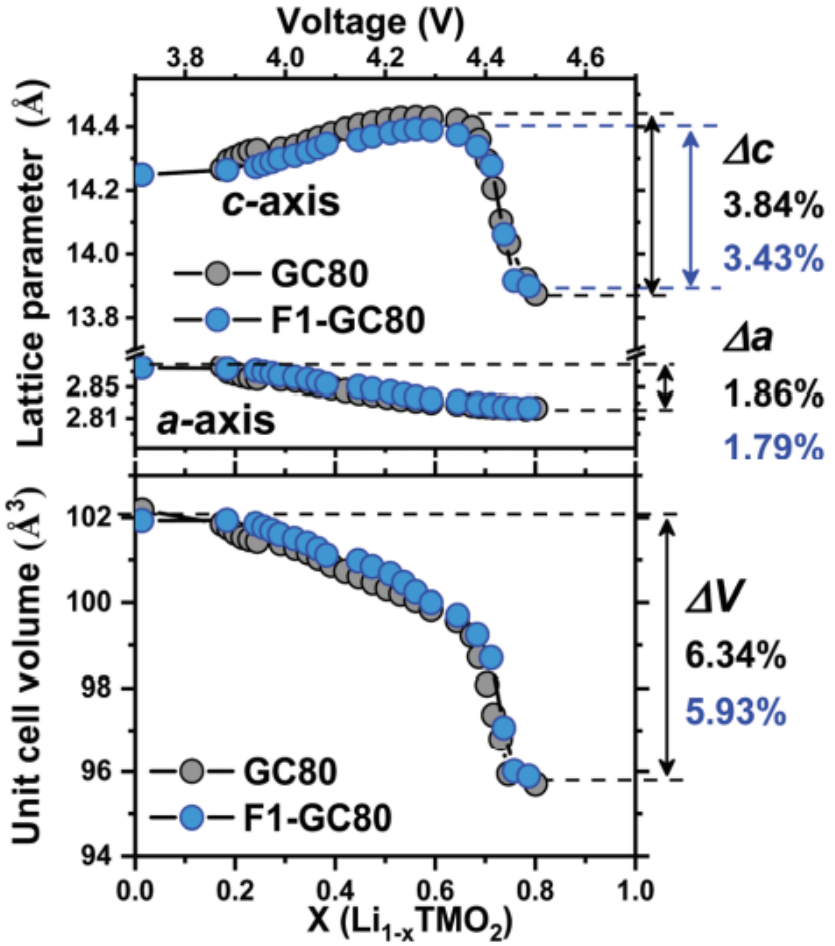
First published: 02 November 2018 | https://doi.org/10.1002/aenm.201802586

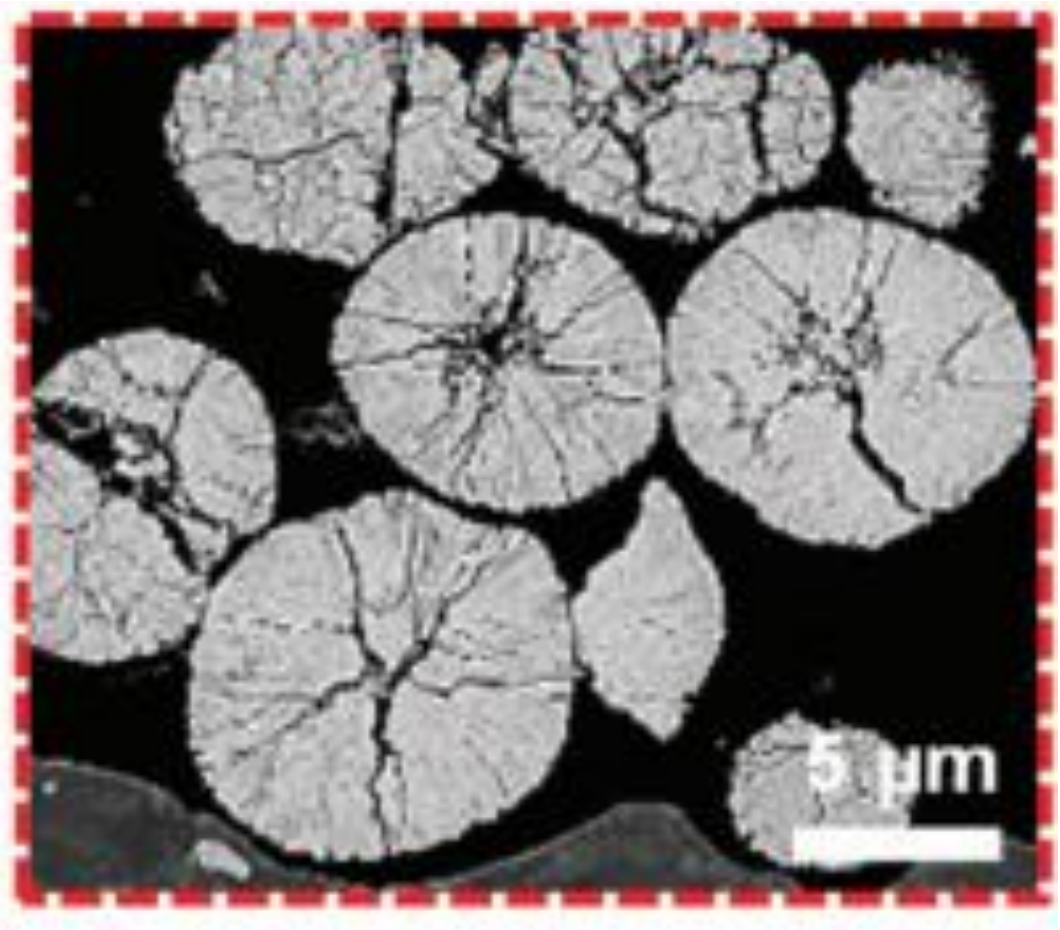


"SURFACE-STABILIZED $LINIO_2$ AS HIGH-CAPACITY CATHODE FOR LI ION BATTERIES"
PCT/US2020/068440



Mechanical strain and NiO phase toward oxygen evolution



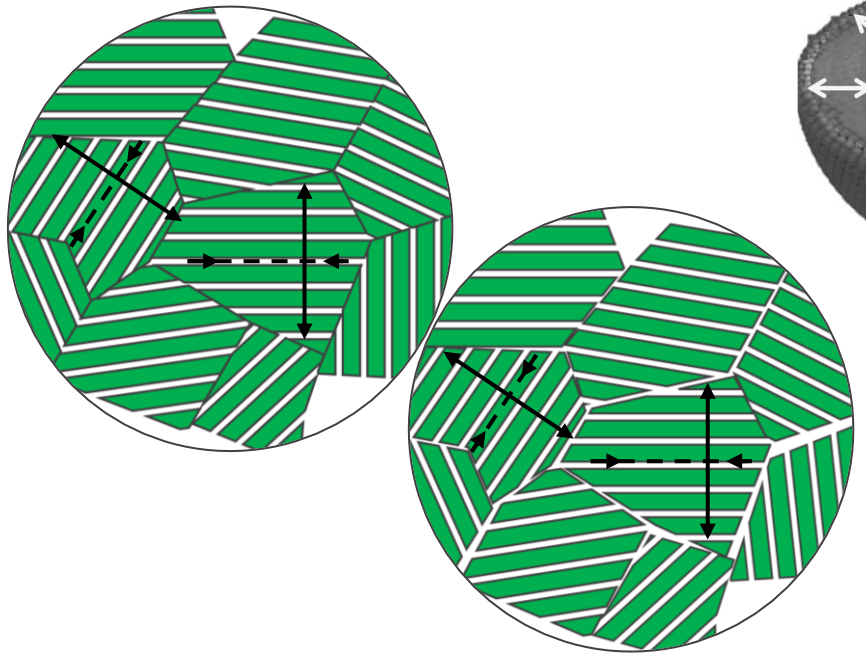


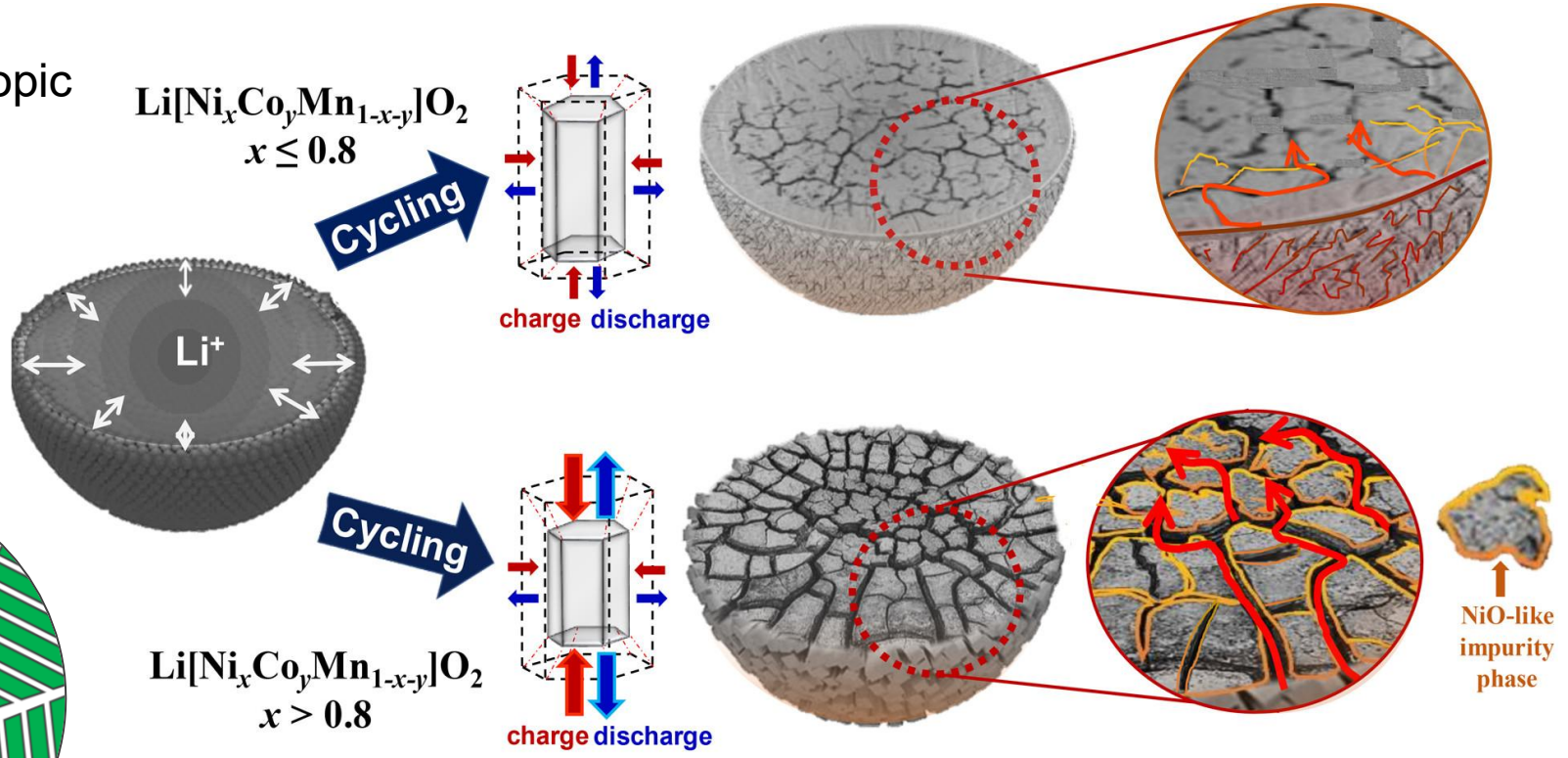
Cho (UTD) – Sun (HYU) collaboration

Energy Environ. Sci., 2021, **14**, 1573–1583

High-Ni polycrystalline NCM pulverization

Mechanical instabilities and anisotropic structural changes, exacerbating surface degradation

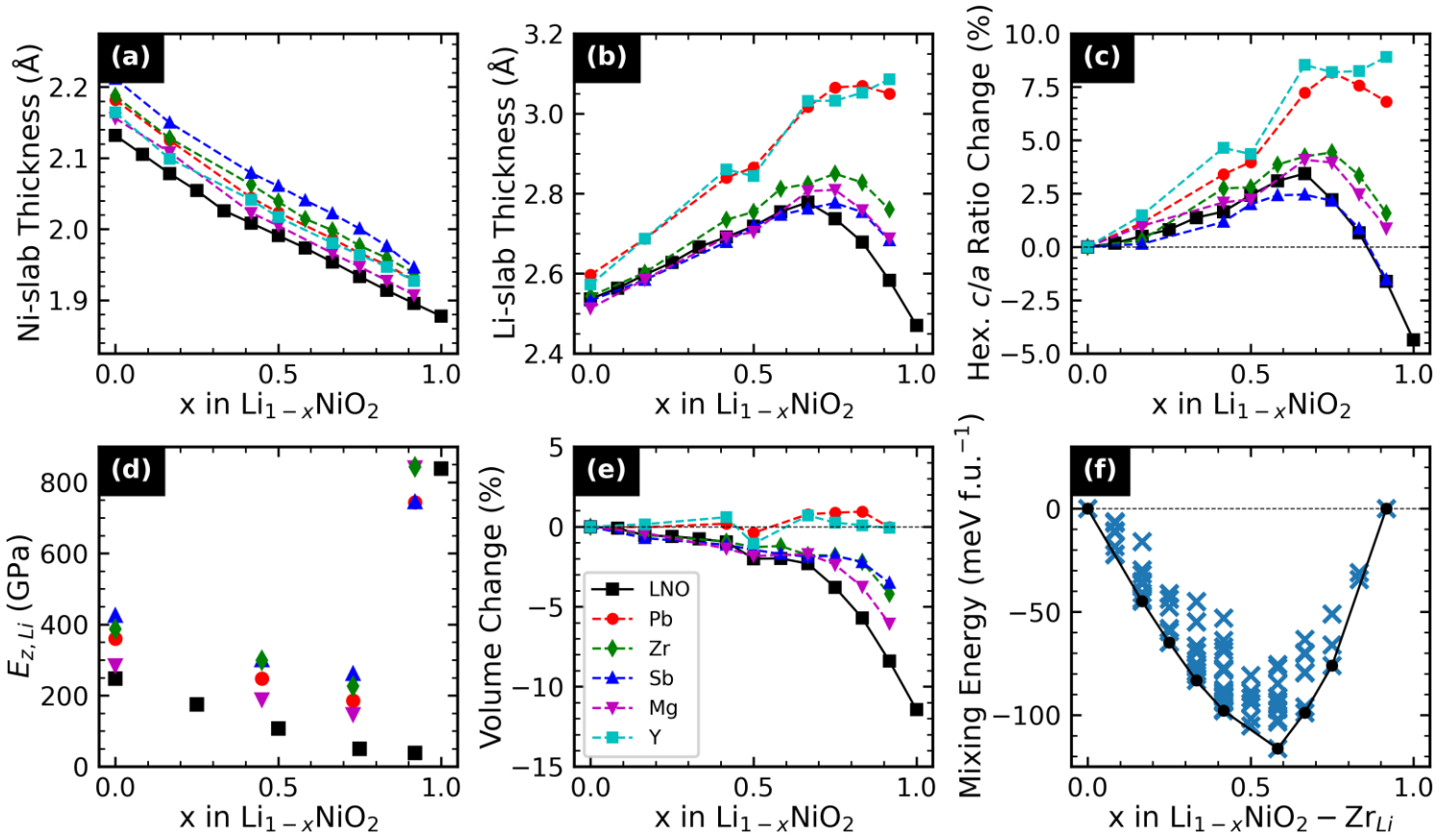


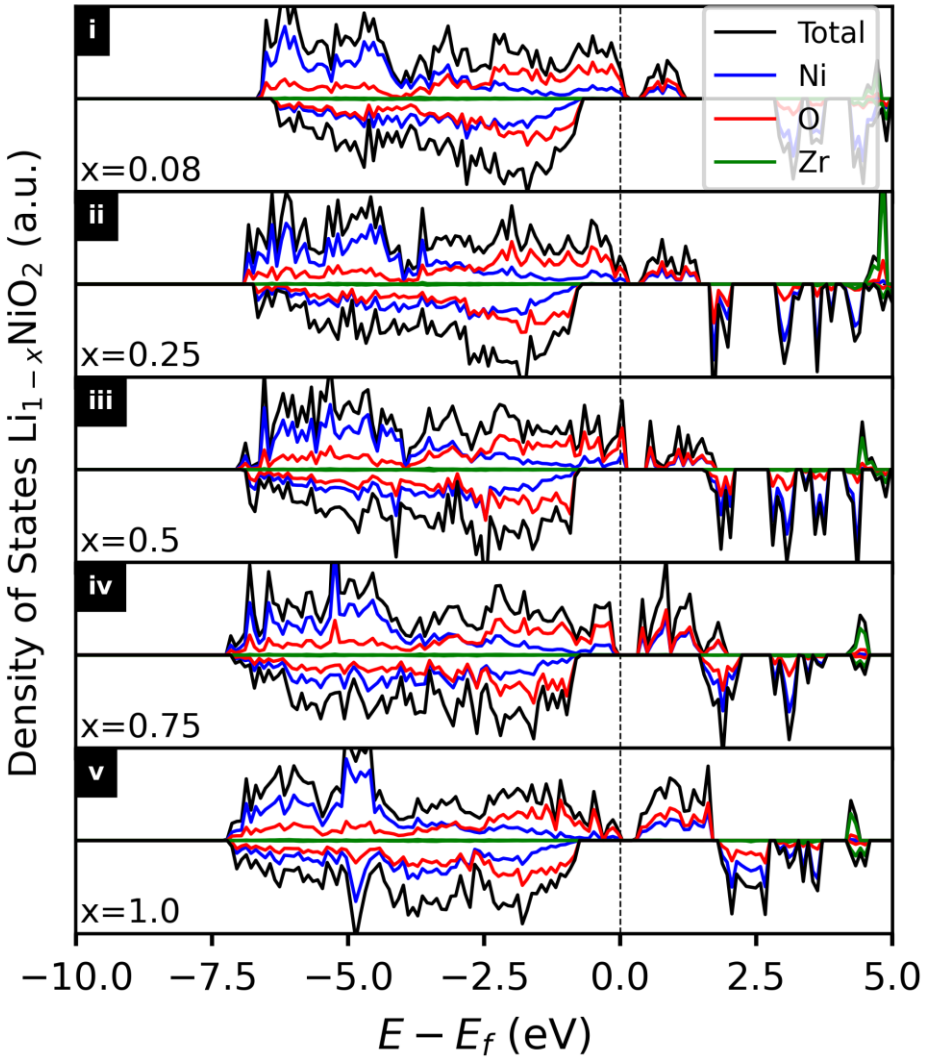


- **Microcrack** from stress-causing anisotropic change
- **Electrolyte Penetration** accelerates the surface degradation along the microcrack

Interlayer (Li-slab thickness (b)) bolstered; volume change lessened; no H2/H3 seg./sep.

Pillaring: M_{Li} (M = Zr, Mg, Sb, Y, Pb)





Rational Design of Battery Cathode Materials to Battery Cell Prototyping at BEACONS

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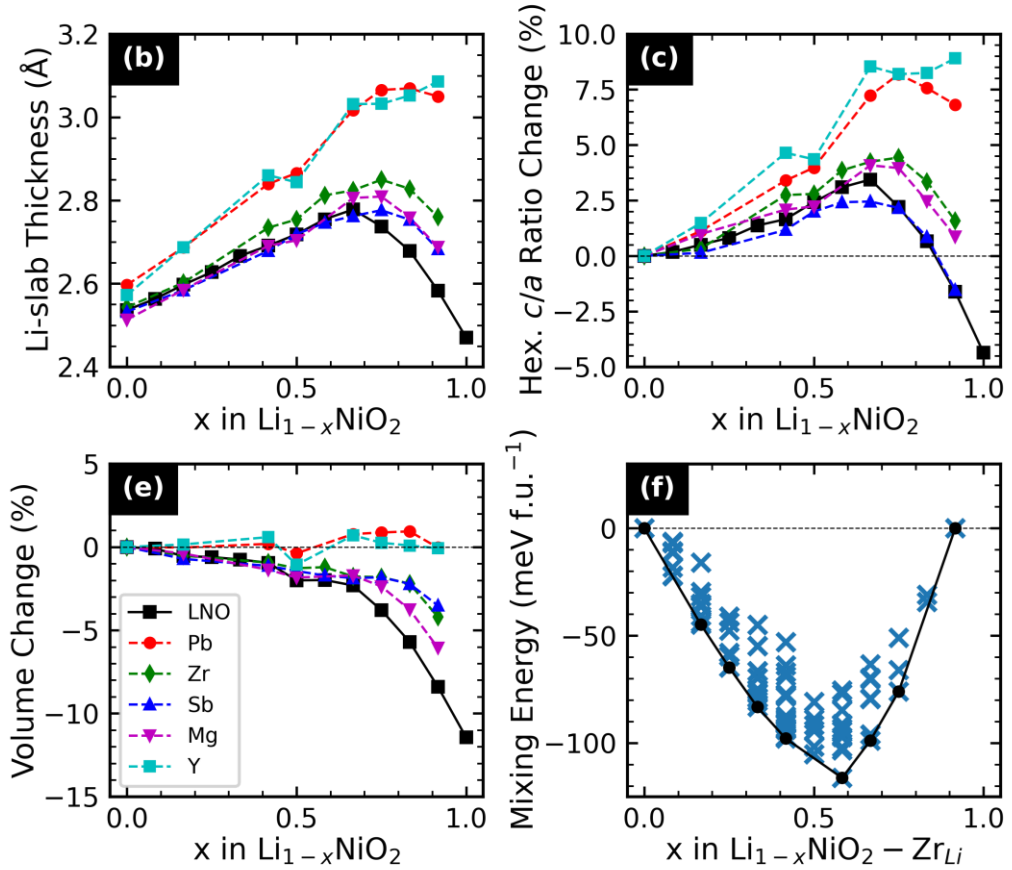
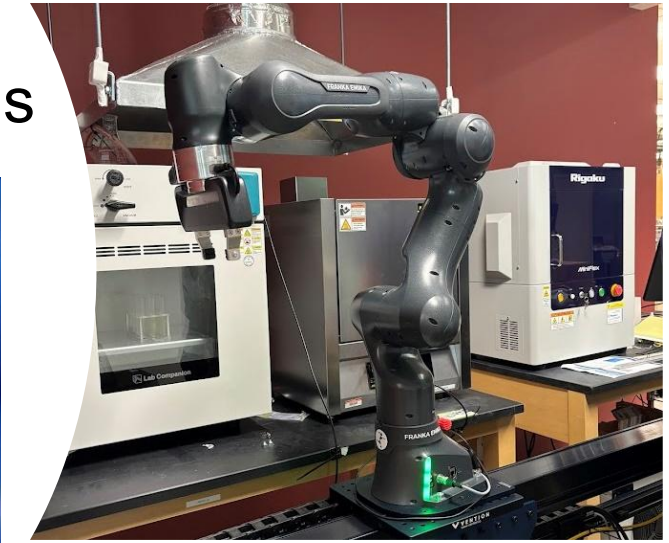


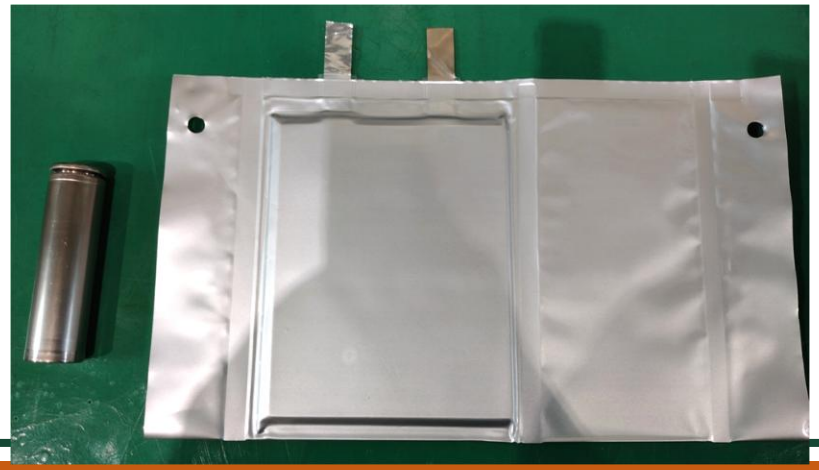
AI/ML
LLM

High-throughput
Robotic synthesis



G2K
Lab

Synthesis
scale-up and
cell prototyping
at BEACONS



Welcome to contact us for follow-up discussions and BEACONS facility information.

kjcho@utdallas.edu

Support

Manufacturing Capability Expansion and Investment Prioritization office within the Department of Defense.

Associated the DOD Scaling Capacity and Accelerating Local Enterprises (SCALE) program, an initiative to create sustainable technologies that support our national security efforts.