NMC811-IQ — Validation Reference

For technical discussions with battery and materials researchers. Each section stands alone and can be excerpted directly.

At a glance

NMC811-IQ is validated at the level of its output: the quantum observables and connected microstate trajectories the dataset publishes. Validation runs on the full-span partner master seams (1–99% lithiation, both charge and discharge) and covers four areas — observable reproducibility, structural-transition positioning, ion-mobility behavior, and charge/discharge symmetry.

What this establishes, in one sentence a researcher can check against data they already have access to: **the published observables faithfully and reproducibly reflect their source states, and the structural and mobility behavior along the trajectories lands where the NMC811 literature says it should, within the variance the field itself reports.**

The generation method — the simulation engine and its circuit design — is proprietary and not disclosed. What is open is everything about the output and how it was validated, which is what matters for evaluating the data.

What is and isn't claimed

Stating this distinction up front tends to shorten technical conversations rather than lengthen them.

Claimed — and demonstrable on the partner master seams:

- The structural turnover associated with the high-state-of-charge phase change appears on both the delithiation and lithiation trajectories, at the lithium content the literature associates with it.
- An independent mobility analysis points at the same transition locations the structural analysis found — two separate methods agreeing on where the transitions are.
- The published observable values reproduce from their source states under the dataset's own computation, on sampled frames, within tight tolerance.

Not claimed:

- A blanket “matches experiment” assertion. The dataset is one probe of NMC811; external measurements are different probes. The comparison is characterized honestly, including where it diverges, rather than asserted as a universal match.
- Reproducibility of the structural-turnover anchor on the public web viewer segments. The relevant lithium-content window sits in the gap between the two public ranges, so the public viewer demonstrates connectivity and partial-range behavior; the full turnover validation is on the partner master seams (available to qualified prospects on request).

How the comparison axis works

Two coordinates appear in the validation: **lithium fraction (x)** — how much lithium is in the lattice — and **cell state of charge (SOC)** — a derived percentage.

Lithium fraction is the material's own coordinate and is the primary axis for any comparison: it is what the structural literature reports against, and it does not depend on how a state was generated. Cell SOC is a derived readout reported alongside x as a secondary. Where both are given, x is the one to weigh first.

This matters for one headline result. The charge/discharge symmetry (the “mirror”) of the high-SOC transition co-locates between the two trajectories to within **0.004 in lithium fraction** and within **~1% in cell SOC** on the best-matched observable pair. Both numbers are reported; the lithium-fraction figure is the one anchored to the material.

Where the structural transition lands

The diffraction and muon-spectroscopy literature places the high-SOC structural turnover of NMC811 — the interlayer-spacing contraction tied to capacity-limiting behavior — at roughly **70–75% cell SOC** (deep delithiation, low lithium content).

The NMC811-IQ structural turnover lands within approximately **5–8% cell SOC** of that center. That offset is reported, not absorbed: it is small, it is in the expected direction, and whether it reflects genuine probe-specific behavior or a calibration detail is exactly what the ongoing characterization examines rather than assumes away. The result sits close to the literature center, on the correct end of the composition range.

The four validation phases

Run as a single orchestrated pipeline; each phase has an explicit pass flag. All currently pass on the latest full run.

Phase 1 — Preliminary. Sanity-checks the SOC axes, confirms the expected transition signal appears on the correct (deep-delithiation) end rather than the wrong end, and audits for confusion between the coordinate axes. A cheap gate that catches gross problems before the deeper phases run.

Phase 2 — Structural turnover. The primary structural claim. Requires the high-SOC transition to appear, with the correct rise-then-fall (charge) / fall-then-rise (discharge) shape, inside the expected transition window on both trajectories — and requires the charge/discharge mirror to co-locate within tolerance. Shape and position are tested separately, and the search is restricted to the regime window so an unrelated, larger feature elsewhere on the trajectory cannot masquerade as the result.

Phase 3 — Mobility proxy. Tests ion-mobility behavior and checks that the points where mobility-related observables diverge line up with the transition locations Phase 2 found independently. Two different analysis pipelines pointing at the same locations is difficult to produce by tuning a single criterion. Includes a null control: an observable with no physical reason to track mobility is run through the same test and must fail it, confirming the test discriminates rather than passing everything.

Phase 4 — Recompute integrity. Confirms the published observable values reproduce from their source states under the dataset's own computation. Tested to tight tolerance on a stratified frame sample. The check itself was verified to detect deliberately injected errors and a known historical computation bug, so a clean pass means genuine agreement between independent computations — not a value compared to itself.

Validation tiers (how the gates are weighted)

- **Tier A — Shape and Mirror:** the gating checks. Correct transition shape in the regime window on both trajectories, and charge/discharge co-location. These determine pass/fail.
- **Tier B — Regime attribution:** which phase boundary a feature belongs to. Informational.
- **Tier C — Position bonus:** how close the turnover sits to the regime center. Reported.
- **Tier D — Axis audit:** cross-checks the coordinate axes against each other. Diagnostic.

The design principle is **shape before position**: a feature has to look like the right kind of transition before its location is even scored, so a correctly-placed feature of the wrong character does not pass.

Falsifiability controls

These are the design choices that make a pass mean something.

- **Band-restricted analysis** — transition scoring runs only inside the expected window, so the largest feature elsewhere on the trajectory cannot dominate the result.
- **Shape tested before position** — the rise/fall character must be correct before location is scored.
- **Single-observable vs. composite separated** — results from individual observables are flagged distinctly from any blended score, so a composite cannot pass on the strength of one dominant term without that being visible.
- **Charge/discharge mirror** — the same feature must appear on both trajectories and co-locate; hysteresis is tolerated as offset, not as disappearance.
- **Cross-pipeline co-location** — the structural analysis (Phase 2) and the independent mobility analysis (Phase 3) must point at the same transition locations.
- **Null control with discriminability** — an unrelated observable must fail the mobility shape test; the real proxies must clear a minimum prominence above it.
- **Recompute discriminator-tested** — the integrity check was confirmed to catch injected errors and a real past bug before its clean result was accepted.
- **Tolerance with external basis** — the comparison tolerance derives from the variance the published NMC811 benchmark literature itself exhibits, not from an arbitrary cutoff.

Scope summary

	Partner master seams (full 1–99%)	Public web viewer segments
Structural turnover, both trajectories	Validated	In coverage gap — not reproducible publicly
Mobility/structure co-location	Validated	Not on public clips
Observable reproducibility	Validated on sampled frames	—
Connectivity, partial-range behavior	Validated	Demonstrable live in viewer

A qualified prospect can request access to the full partner master seams to reproduce the structural and mobility validation directly.

References

The structural and mobility comparisons above are checked against the following peer-reviewed literature. DOI links resolve directly to the publisher record.

Primary reference

Märker, K.; Reeves, P. J.; Xu, C.; Griffith, K. J.; Grey, C. P. “Evolution of Structure and Lithium Dynamics in $LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$ (NMC811) Cathodes during Electrochemical Cycling.” *Chemistry of Materials* 2019, 31 (7), 2545–2554.

DOI: 10.1021/acs.chemmater.9b00140. Methods: operando synchrotron XRD, electrochemistry, and ex situ solid-state NMR. Supports the interlayer-spacing (c-axis) contraction at high SOC and the rise-then-drop in lithium mobility across the high-SOC region cited above.

Supporting references

McClelland, I.; Booth, S. G.; Anthonisamy, N. N.; Middlemiss, L. A.; Pérez, G. E.; Cussen, E. J.; Baker, P. J.; Cussen, S. A. “Direct Observation of Dynamic Lithium Diffusion Behavior in Nickel-Rich, $LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$ (NMC811) Cathodes Using Operando Muon Spectroscopy.” *Chemistry of Materials* 2023, 35 (11), 4149–4158.

DOI: 10.1021/acs.chemmater.2c03834. Operando muon spectroscopy (μSR) measuring bulk Li^+ ion mobility across the first charge/discharge cycle. Finds Li^+ diffusion faster at higher state of charge — the directional mobility behavior the NMC811-IQ mobility-proxy phase tests against.

Wu, F.; Liu, N.; Chen, L.; Su, Y.; Tan, G.; Bao, L.; Zhang, Q.; Lu, Y.; Wang, J.; Chen, S.; Tan, J. “Improving the reversibility of the H2–H3 phase transitions for layered Ni-rich oxide cathode towards retarded structural transition and enhanced cycle stability.” *Nano Energy* 2019, 59, 50–57.

DOI: 10.1016/j.nanoen.2019.02.027. Mechanism reference for the H2→H3 transition in Ni-rich layered oxides (study system: $LiNi_{0.9}Co_{0.1}O_2$): abrupt c-axis lattice contraction, anisotropic volume change, and capacity fade tied to loss of the H3 phase. Cited for the general Ni-rich mechanism, not as an NMC811-specific measurement.

Comparison tolerances throughout this document derive from the spread across these published sources. Additional references are available on request.

Validation covers output fidelity and behavior against published NMC811 structural and mobility data. The simulation method is proprietary by design; the value of the dataset does not depend on its disclosure, and every claim above is checkable against the output itself.