ARRADIANCE *Sneak Preview*

Mitigating First-Cycle Capacity Losses in NMC811 via Lithicone Layers by MLD

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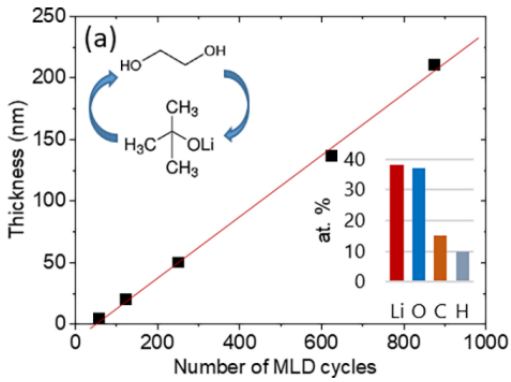
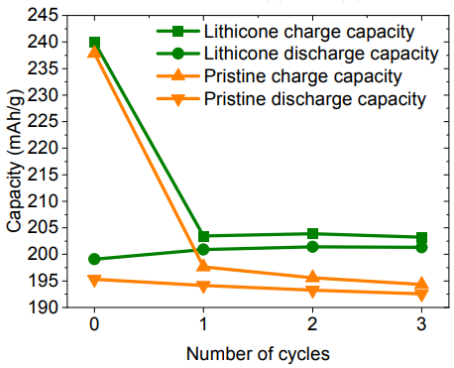
Nickel-rich Li-Ni-Mn-Co (NMC811) electrodes represent one of the most promising cathode materials for high-energy-density automotive lithium-ion batteries. Capacity and the energy density of these batteries may be increased significantly by mitigating the so-called *first-cycle capacity loss*. The origin of this capacity loss is likely due to a combination of (1) loss of lithium due to irreversible reactions with the electrolyte, (2) loss of active cathode material due to irreversible structural changes, and (3) slow kinetics close to the discharged state.

This new report by scientists from the Swiss Federal Laboratories for Materials Science and Technology (EMPA) highlights that capacity losses associated with (1) and (2) may be mitigated by creating an artificial cathode electrolyte interphase (CEI) layer. They employed molecular layer deposition (MLD) to grow lithicone layers directly onto porous NMC811 particle electrodes. In this work, lithicone layers were deposited with lithium tert-butoxide (LiOtBu) and ethylene glycol as precursors, in Arradiance GEMStar™ XT-P reactor coupled to an argon-filled glovebox, at a low reactor temperature, to avoid thermal degradation of the electrode binder. Film thickness coverage on Si wafer-based high-aspect ratio structures was found to linearly decline from 210nm to 30-40nm at 20:1 aspect ratio, an important engineering variable to attempt commercialization of this technology. When attempted on actual electrodes, agglomeration of carbon particles (present to provide electronic contact between NMC811 particles) impeded uniform MLD growth, resulting in less lithicone coverage.





*K.Egorov, W.Zhao, et. al., ACS Appl. Mater. Interfaces 2023, 15, 20075−20080

The lithicone-coated electrodes were assembled into electrolytic lithicone/graphite coin cells. Although the electrode with 20nm lithicone shows approximately the same first-cycle charge capacity of 240 mAh/g as the pristine electrode (graph above), it shows a higher second-cycle charge capacity, indicating that lithicone reduces capacity losses during the first cycle by reducing electrolyte decomposition during CEI formation and the consumption of active lithium. Long-term cycling, rate and accelerated ageing tests confirmed improvement in capacity loss reduction. Additional cell capacity/voltage tests indicated that lithicone may act as a benign artificial CEI layer.

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