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Investigating surface sensitivity of Ni-rich cathode material towards CO2 and H2O

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Layered Ni-rich transition metal oxide materials have been considered as the most promising cathode utilized in Li-ion batteries, e.g., LiNi0.8 Mn0.1 Co0.1 O2 (NMC 811). However, one of the drawbacks of NMC 811 is its high air sensitivity, leading to a degradation layer forming on the surface, and a lower cycling performance.[1] Since the degradation mechanism is not fully understood, in this work, we use ambient pressure photoelectron spectroscopy (APPES) [2] to investigate the surface sensitivity of NMC 811 towards CO2 and H2O in situ, aiming to determine the factor triggering the degradation. Before gas exposure, NMC 811 surface was studied in UHV. The changes in surface chemical composition were monitored as a function of time and gas pressure. Results show that carbonate compounds will form on the surface when NMC 811 is exposed to CO2 at around10-3 mbar and start to disappear in UHV after CO2 exposure. More interestingly, the photon beam can accelerate the formation of carbonate on NMC particles surface. The same measurements were finished with H2O exposure as well. Results indicate that lithium hydroxide is formed, where active surface oxygen can be the possible explanation.[3] However, this reaction is reversible in UHV as well.

References
[[1] R. Jung et al., "Effect of Ambient Storage on the Degradation of Ni-Rich Positive Electrode Materials (NMC811) for Li-Ion Batteries," Journal of The Electrochemical Society, vol. 165, no. 2, pp. A132-A141, 2018, doi: 10.1149/2.0401802jes.
[2] E. Kokkonen et al., "Upgrade of the SPECIES beamline at the MAX IV Laboratory," Journal of Synchrotron Radiation, vol. 28, no. 2, pp. 588-601, 2021-03-01 2021, doi: 10.1107/s1600577521000564.
[3] M. Yoon et al., "Reactive boride infusion stabilizes Ni-rich cathodes for lithium-ion batteries," Nature Energy, vol. 6, no. 4, pp. 362-371, 2021-04-01 2021, doi: 10.1038/s41560-021-00782-0.

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