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The Lithium-Induced Conversion Reaction of CoO Thin Film Battery Materials as Studied by ARXPS¹ RYAN THORPE, SYLVIE RAN-GAN, MAHSA SINA, FREDERIC COSANDEY, ROBERT BARTYNSKI, Rutgers Univ — Conversion reaction compounds such as CoO exhibit high charge density as electrodes in Li-ion batteries. Upon exposure to lithium, Co ions are reduced from a 2+ oxidation state to Co^0 in a reaction that drastically changes the electronic structure and morphology of the electrode. In order to characterize the atomistics of this conversion reaction without contamination from electrolytes or ambient gases, we have grown CoO thin films in (100), (111), and polycrystalline orientations, and exposed these surfaces to atomic Li in ultra-high vacuum. The diffusion of Li and the phase evolution of the substrate were then characterized with STM and angle-resolved XPS. Differences in the reactivities of each crystalline face have been observed. Additionally, a parasitic reaction between Li-rich reaction products and residual H₂O was observed to produce Li₂O₂, which inhibited further Li diffusion at room temperature. This could explain the capacity losses observed in CoO electrodes by previous studies.

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Ryan Thorpe Rutgers Univ

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