



DEPARTMENT OF
Chemistry
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Ph.D. Dissertation Defense

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The main drive of this thesis is to understand what material factors influence the biological and environmental impact of emerging nanoscale transition metal oxide materials and to use this knowledge to redesign new materials to have reduced adverse effects. Emerging nanomaterials such as lithium nickel manganese cobalt oxides ($\text{Li}_x\text{Ni}_y\text{Mn}_z\text{Co}_{1-y-z}\text{O}_2$, $0 < x, y, z < 1$, also known as NMC) and lithium cobalt oxide (Li_xCoO_2 , $0 < x < 1$, also known as LCO) technology have increasing complexities to address technological needs. Large scale commercialization of these materials make them potential environmental contaminants through routes of manufacturing, usage, and disposal.

To evaluate the potential impact of nanoscale NMC and LCO on environmental systems, we first synthesized these materials using a two-step process that yielded control over morphology and chemical composition. These nanomaterials were characterized in parallel to biological studies to analyze changes to the surface and bulk composition and solution species. We identified that both NMC and LCO release transition metals in solution in an incongruent manner. Released Ni and Co ions were responsible for either some or most of the toxicity seen from the nanomaterial exposures. There is evidence that suggests the release of transition metals in high oxidation states such as Co^{3+} can cause hydroxyl radical formation and also contribute to observed toxicity. In order to reduce the observed biological impact seen from released Ni and Co, we synthesized NMCs with lower Ni and Co content. This redesign process lowered the toxicity for the gram-negative bacterium, *Shewanella oneidensis* MR-1. In these studies we learned that chemical composition of the nanoscale complex oxides are important in affecting the material's transformation process in aqueous matrices and this can ultimately impact toxicity. This thesis maintains that this chemical transformation insight is crucial in aiding the development of benign-by-design nanoscale cathode materials.

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