First Principle Modeling of $Li_{1-x}Ni_yCo_zAl_{0.50}O_2$ Type Cathode Materials in Lithium Ion Batteries

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By the year 2100, world's population will be 12 billions while the energy consumption will be 1,400 Qbtu/year (report by the United Nations). Rechargeable lithium-ion batteries (LIBs) are the primary choice as energy storage devices. However, the current LIB technology has reached its limits and not adequate for future energy storage needs. Extensive research has been performed in developing novel anode materials. However, design of cathode materials plays a crucial role in over-all performance of LIBs. One of the important characteristics of the cathode materials is its good intercalation behavior. $LiCoO_2$ (LCO) and $LiNiO_2$ (LNO) are the well-studied cathode materials. LCO has low thermal stability due to the exothermic release of oxygen when heated over a certain point. LNO has structural instability during charging process due to Li/Ni cation mixing. One strategy that holds promise is to dope LNO with other transitional metal atoms in order to reduce cationic disorder. Small amount of Co-doping and a very little amount of Al-doping helps improve both the thermal instability and electrochemical properties of LNO. In this regard, $Li_{1-x}Ni_yCo_zAl_{0.50}O_2$ (NCA) cathode achieves ubiquitous commercial success due to its high useable discharge capacity and long storage calendar life. In this work, we considered three different types of NCA materials: $Li_{1-x}Ni_{0.80}Co_{0.15}Al_{0.05}O_2$, $Li_{1-x}Ni_{0.85}Co_{0.10}Al_{0.05}O_2$, and $Li_{1-x}Ni_{0.90}Co_{0.05}Al_{0.05}O_2$ (x ranges from 0 to 1). Our results suggest that with the decreasing Co concentration, the overall thermodynamic potential decreases. The higher Co content shifts the Fermi level of the mixed transition metals more near t_{2g} orbitals (from e_g) and this accounts for the higher thermodynamic potential. In order to get more insight into our results, we propose to investigate phase changes in cathode materials during charging process (extraction of Li). In addition, incorporation of other metals, especially Na in NCA is known to enhance electrochemical properties. We also propose to study specific role of other metal incorporation in NCA. Our work will help design better cathode materials and improve the overall efficiency of LIBs.

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