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Effect of Transition Metal Ordering on the Electronic Properties of $LiNi_{1-y-x}Co_yMn_xO_2$ Cathode Materials for Li-ion Batteries[1] ROBERTO LONGO, FANTAI KONG, SANTOSH KC, University of Texas at Dallas, USA, DONG-HEE YEON, JAEGU YOON, JIN-HWAN PARK, SEOK-KWANG DOO, Samsung Electronics, Republic of Korea, KYEONGJAE CHO, University of Texas at Dallas, USA, MSL TEAM, SAIT TEAM — Current Li-ion batteries use layered oxides as cathode materials, specially $LiCoO_2$ or $LiNi_{1-y-x}Co_yMn_xO_2$ (NCM), and graphite as anode. Co layered oxides suffer from the high cost and toxicity of cobalt, together with certain instability at high operational temperatures. To overcome these difficulties, the synthesis of novel materials composed of layered oxides with different sets of Transition Metals (TM) has become the most successful way to solve the particular drawbacks of every single-oxide family. Although layered materials can deliver larger capacity than other families of cathode materials, the energy density has yet to be increased in order to match the expectations deposited on the NCM oxides. To acquire a high capacity, they need to be cycled at high operational voltages, resulting in voltage and capacity fading over a large number of cycles. In this work, we examine the phase diagram of the Li-Ni-Co-Mn-O system and the effect of TM ordering on the electronic properties of NCM cathode materials, using density-functional theory. Our findings will provide conceptual guidance in the experimental search for the mechanisms driving the voltage and capacity fading of the NCM family of cathode materials, in an attempt to solve such structural instability problems and, thus, improving the performance of the NCM cathode materials.

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Roberto Longo
University of Texas at Dallas

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