Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Dopant based stabilization of $LiCoO_2$[1]

JUAN A. SANTANA, JEONGNIM KIM, FERNANDO A. REBOREDO, Materials Science and Technology Division, Oak Ridge National Laboratory, PAUL R. KENT, Center for Nanophase Materials Sciences and the Computer Science and Mathematics Division, Oak Ridge National Laboratory —

$LiCoO_2$ is still one of the commonly used cathode materials for Li-ion batteries. Yet, the usable specific capacity is limited to approximately 150 mAh/g, only above half of its theoretical capacity (280 mAh/g). The limitation arises predominantly from the decomposition (or mechanical failure) of the $LiCoO_2$ cathode into Co_3O_4 when more than 50% of Li is deintercalated. The stability of the cathode and its electrochemical performance can be improved by coating the cathode surface with inner metal oxides. This approach has been widely used for different cathode materials, but the origin of the stabilization effect is poorly understood. Various models have been proposed to rationalize the stabilization, e.g., *i*) the inner metal oxides act as a physical barrier preventing cathode-electrolyte reactions, and *ii*) the layered structure of the cathode material is stabilized by the migration of metal ions from the coating oxides. To elucidate the origin of the higher stability, we have performed first-principles DFT calculations of $LiCoO_2$ when doped with inner metal ions. Our calculations explore the effect of the dopants on the formation of point defects and the thermal decomposition of the cathode electrode.

[1] Research supported by the U.S. Department of Energy, Basic Energy Sciences, Materials Sciences and Engineering Division

Juan A. Santana
Oak Ridge National Laboratory

Date submitted: 14 Nov 2013

Electronic form version 1.4