

## **Seminar**

# **What happens when Ni-rich Li-ion cathode materials lose oxygen during charge-discharge process?**

**Hena Das**

**Cornell University, NY**

Layered Ni-rich complex oxides, such as  $\text{LiNi}_{0.8}\text{Co}_{0.15}\text{Al}_{0.05}\text{O}_2$  (NCA) and  $\text{LiNi}_x\text{Mn}_{x'}\text{Co}_{(1-x-x')}\text{O}_2$  (NMC) are popular choices as cathode materials for lithium-ion rechargeable batteries because of their high energy density. However, Ni-rich materials show a rise in impedance when charged to high voltages, which is, reportedly, triggered by surface phase transformation of these materials from layered to disordered spinel-like and/or rock-saltlike structures, conjectured to occur due to oxygen loss followed by cation densification. Despite several reports on the surface phase transformations the precise structures and compositions of these surface phases are unknown. We, for the first time address this problem using first principles theoretical techniques. Here, I will discuss the thermodynamic phase equilibria as a function of transition metal ion content in the cathode material in the context of lithium nickel oxides. Our investigations predict the existence of several Ni-rich phases that are, to date, unknown in the scientific literature and can significantly contribute towards the observed increase in ionic impedance.

***Wednesday, Jan 24<sup>th</sup> 2018***

***04:00 PM (Tea/Coffee at 03:30 PM)***

***Seminar Hall, TIFR-H***