

## Studies of Cathode Materials for Lithium-Ion Batteries in Bar-Ilan University: Recent Advances and Challenges

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We present in this work the recent studies in Bar-Ilan University of materials for positive electrodes of Li-ion batteries. The focus is on the lithiated oxides of Ni-rich  $\text{Li}[\text{Ni}_x\text{Co}_y\text{Mn}_z]\text{O}_2$  family (NCM,  $R\text{-}3m$  space group),  $x=0.5\text{-}0.8$ . The main questions studied were lattice doping by  $\text{Al}^{3+}$ ,  $\text{Zr}^{4+}$  and  $\text{Mo}^{6+}$  of the above materials in relation to the electrode behavior, structural stability, and thermal reactions [1,2]. For these materials, using density functional theory calculations, we have shown that doping by the above cations is preferred at Ni sites. It was established that the interfacial resistance of the doped samples is much lower compared to that of undoped measured at several potentials during charge. For these electrodes, the interfacial resistance increases rapidly with cycling, while Zr and Mo-doped electrodes exhibit stability of this parameter even at high electrode potentials,  $>4.0$  V, upon cycling. This implies therefore more stable modified electrode/solution interface of doped electrodes developed on these samples. We discuss also the following issues: *ab-initio* calculations of the preferential substitution of  $\text{Al}^{3+}$ ,  $\text{Zr}^{4+}$  and  $\text{Mo}^{6+}$  on the Li or transition metal sites; influence of dopant ions on the  $\text{Li}^+/\text{Ni}^{2+}$  mixing and on charge distribution, changes of the lattice constants, voltage profiles, and of the dopant segregation at the surface (studied by TOF-SIMS, EXAFS, HAADF-STEM). Special attention is paid also on partial layered-to-spinel structural transformation of  $\text{Li}[\text{Ni}_x\text{Co}_y\text{Mn}_z]\text{O}_2$  electrodes during cycling and on thermal characteristics in reactions with solutions. A possible mechanism of the above transformation in Ni-rich NCMs is proposed (based on the computational studies) that includes irreversible migration of Ni-ions in  $\text{Li}[\text{Ni}_x\text{Co}_y\text{Mn}_z]\text{O}_2$  electrodes upon the  $\text{Li}^+$  deintercalation.

### References:

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