

Aluminum Distribution in the Pristine NCA Cathode

Scientific Achievement

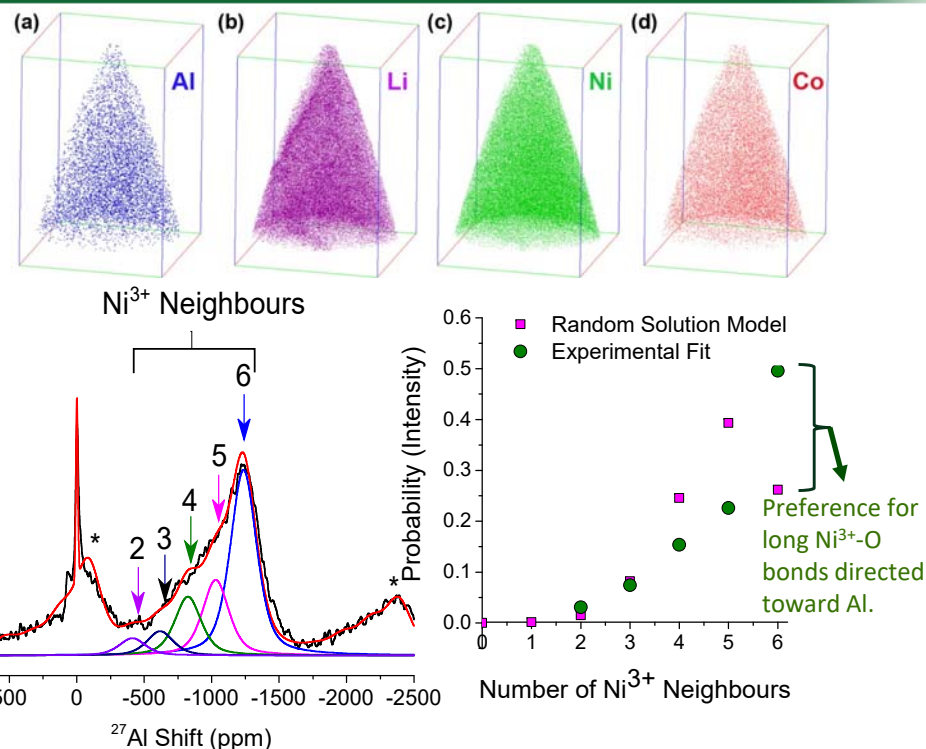
Assignment of the ^{27}Al NMR shifts using insights from DFT and APT indicates a preference for lengthened Jahn-Teller Ni-O bonds to be orientated towards the Al in pristine $\text{LiNi}_{0.8}\text{Co}_{0.15}\text{Al}_{0.015}\text{O}_2$ (NCA).

Significance and Impact

Provides further insight into the role that Al plays in stabilizing the transition metal layer in doped- LiNiO_2 .

Research Details

- ^{27}Al and ^7Li NMR were performed to investigate the Al distribution in NCA.
- NMR shift calculations combined with DFT structural calculations were used to assign the ^{27}Al NMR shifts in a paramagnetic environment (near Ni^{3+}).
- Atom probe tomography was performed to confirm the homogenous distribution of cations in bulk NCA.



Findings: Al is homogenously distributed in the bulk NCA. NCA experiences a dynamic Jahn-Teller distortion. Although still a dynamic JT distortion, the lengthened JT Ni^{3+} -O bond is preferentially directed towards the Al atom. This preferential ordering of the lengthening of the JT Ni^{3+} -O bonds may lead to a stabilization of the metal layer.

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