NMC Core-Shell: characterizing the future of Li-ion battery cathodes

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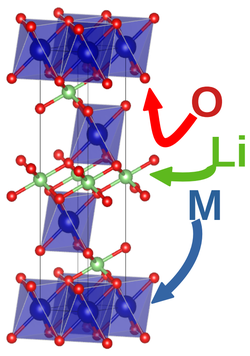
Motivation

The popularization of electric vehicles, the expected rise in the number of batteries inside commercial devices and the increasing demand of energy storage due to renewable energies are some of the reasons for the increase in relevance of Li-ion Batteries (LIBs). Due to the high demand, different approaches are being pursued in order to improve LIBs. One key factor is the stability of the different parts present in the battery, especially the cathode. Here an study of the crystal structure and morphology of microparticles of NMC, a widely used cathode material, with core-shell structure is presented.

NMC: Li-Ni-Mn-Co-O



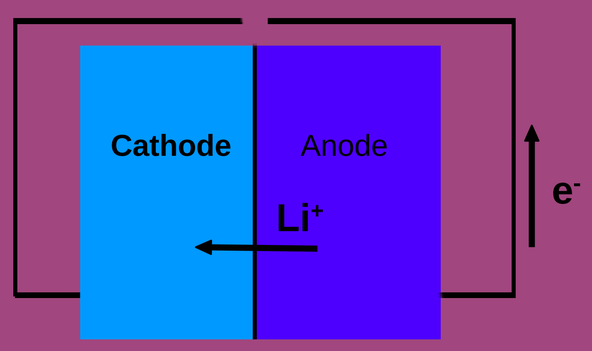
$LiMO_2$ – stacked oxides (R-3m)[1]

- **Ni**: High Capacity
- **Mn**: Structural Stability
- **Co**: Reduce Cation Disorder

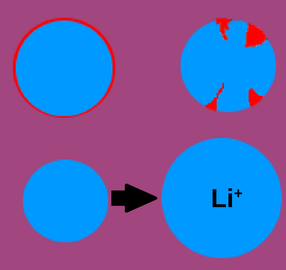
$LiNi_xMn_yCo_{1-x-y}O_2$

NMC 811: 80% Ni, 10% Mn, 10% Co

NMC cathodes: difficulties[2]



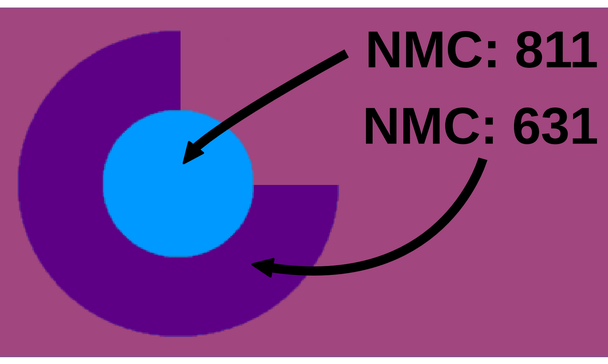
Cathode Particles



- Lattice expansion
- Surface reconstruction
- Surface stabilization
- Cracks on particles

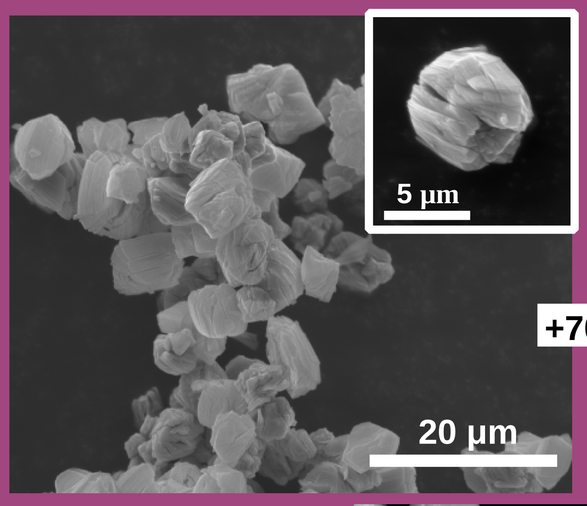
Solution: NMC Core-Shell microparticles

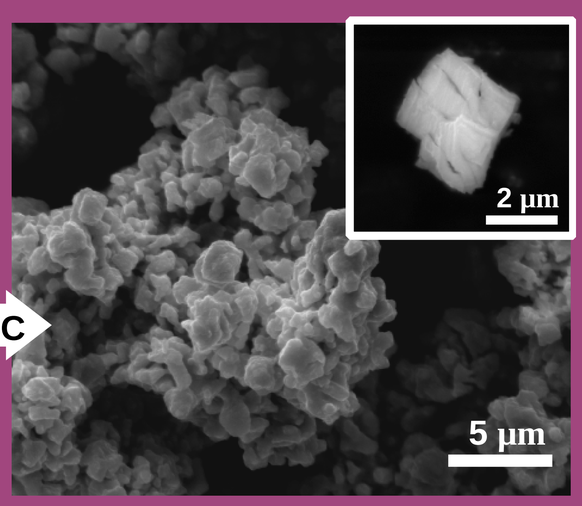
Microparticles	Core-Shell	Stacked Oxides
▪ High Surface/Volume ▪ Short diffusion paths ▪ Controllable ΔV	▪ Rich Ni Core: High Capacity ▪ Rich Mn shell: Less effect of ΔV	▪ Easier introduction/extraction of Li ▪ Lower loss of Li ▪ Stable crystal structure: stable particles

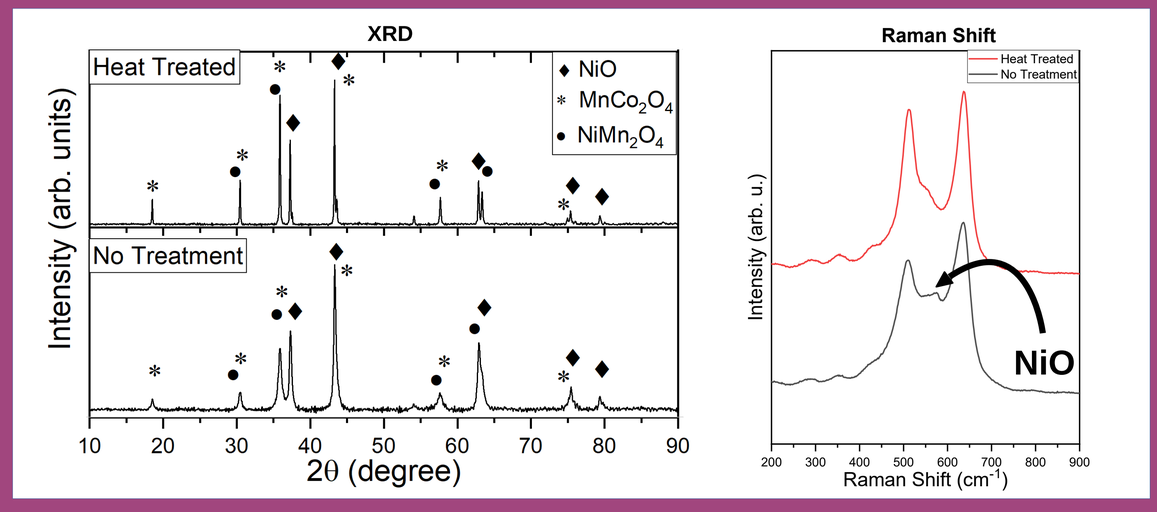


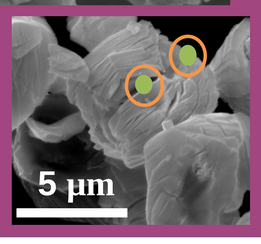
Core-Shell no Li

Chemical synthesis ➡ Core: dried at 110 ºC/60 min + Shell: dried at 110 ºC/60 min + Heat treatment: **500 ºC/2h** / **500 ºC/2h + 700 ºC/2h**









Core-Shell: 4 µm
Shell: 0.5 - 1 µm

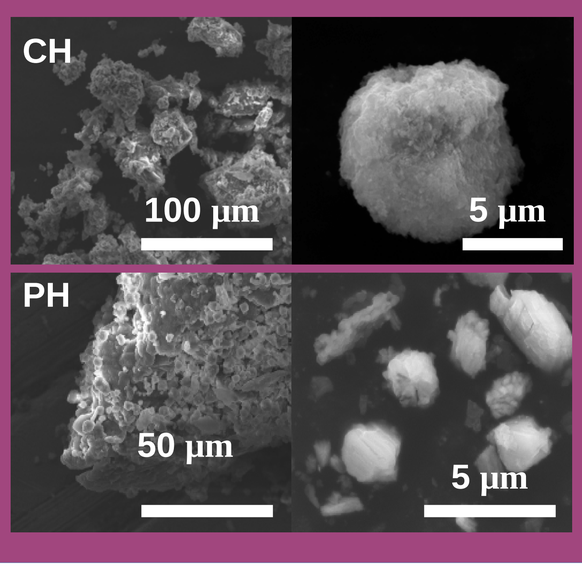
+

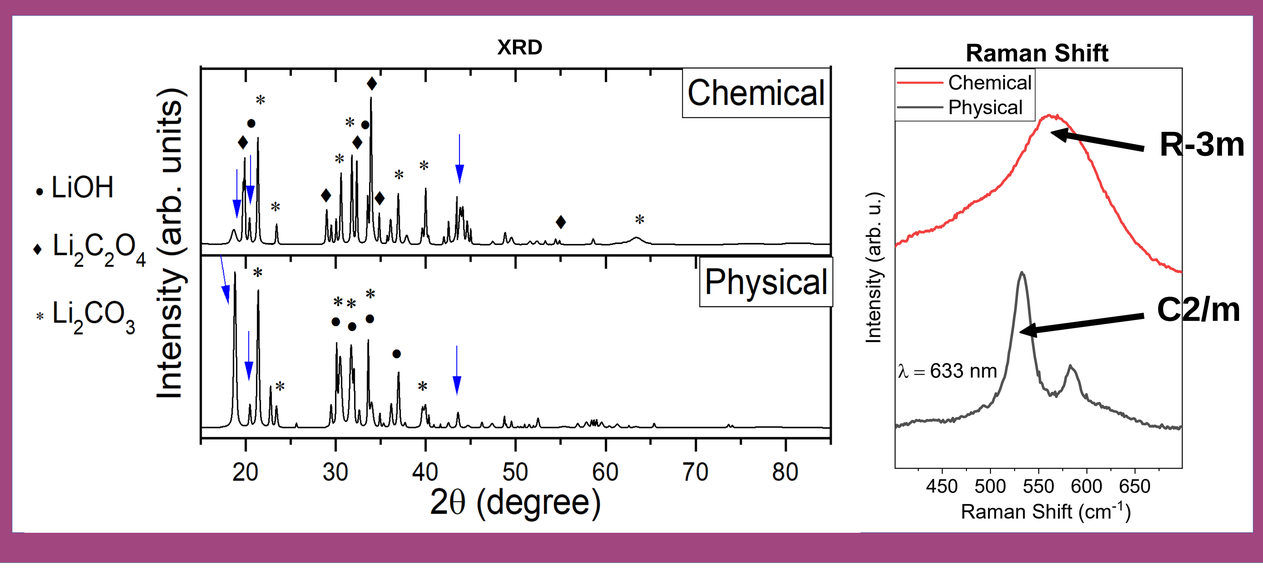
- $NiMn_2O_4$ and $MnCo_2O_4$
- NiO
- Higher T: **-** NiO and **+** $NiMn_2O_4$

➡ **Core-Shell Cation mixing**

Li introduction

Physical (Top-Down) approach ➡ Core-Shell particles milled with Li compounds and heat treated
Chemical (Bottom-Up) approach ➡ Li through solution evaporation Core + Shell + Heat treated (350 - 700 ºC)





Physical:
- No Core-Shell
- Little Li introduction
- No layered oxides

Chemical:
- **Core-Shell**
- **Li** introduction
- **Layered structure** (R-3m)[3] at high temperatures

References

1. Xu, J., Lin, F., Doeff, M. M., & Tong, W. (2017). A review of Ni-based layered oxides for rechargeable Li-ion batteries. Journal of Materials Chemistry A, 5(3), 874-901.
2. Li, T., Yuan, X. Z., Zhang, L., Song, D., Shi, K., & Bock, C. (2020). Degradation mechanisms and mitigation strategies of nickel-rich NMC-based lithium-ion batteries. Electrochemical Energy Reviews, 3(1), 43-80.
3. Ruther, R. E., Callender, A. F., Zhou, H., Martha, S. K., & Nanda, J. (2014). Raman microscopy of lithium-manganese-rich transition metal oxide cathodes. Journal of The Electrochemical Society, 162(1), A98.

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