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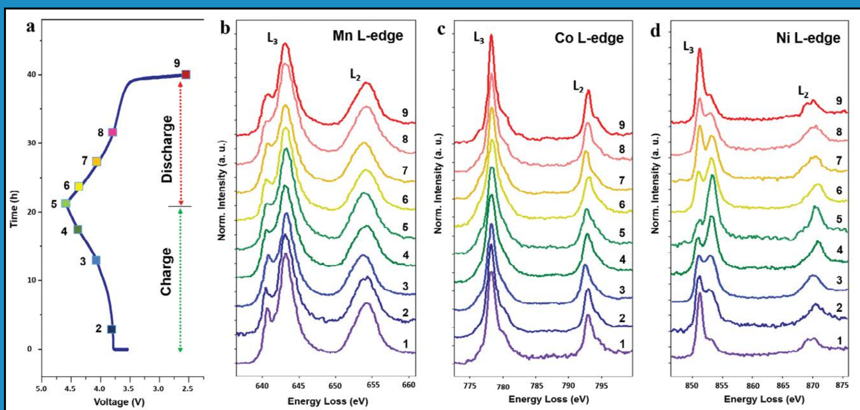
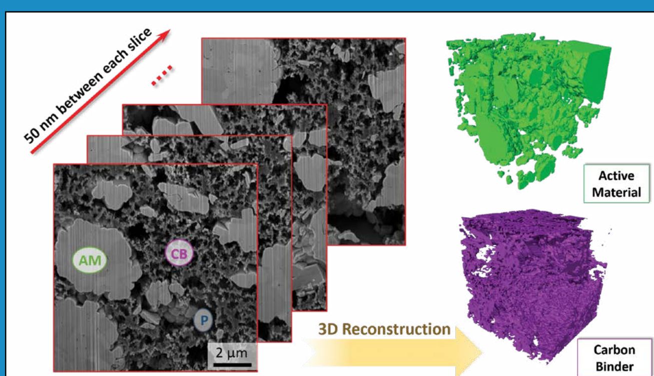
Study on the Chemical and Structural Evolution of Lithium-Ion Battery Cathodes

The rapid development of modern technologies places stringent demands on the improvements of energy density, lifetime, and safety for lithium-ion batteries (LIBs). Whereas, the performance decay mechanisms of the LIBs during electrochemical cycling are not yet fully understood. Herein, state-of-the-art electron microscopy techniques are used to perform an in-depth study on the degradation mechanism of layered lithium transition metal oxide cathodes. Using analytical TEM, the chemical and structural evolution of the cathode materials during cycling is unraveled down to the atomic scale. Beyond 2D characterization, 3D microstructure reconstructions of the LIB cathodes using FIB-SEM serial sectioning, reveal the microstructural changes of different cathodes upon cycling. These studies, therefore, provide valuable guidance for the future design of high-energy-density cathodes.



Investigation of the charge compensation mechanism and structural evolution of LiNi1/3Mn1/3Co1/3O2 cathode material during electrochemical cycling using EELS.



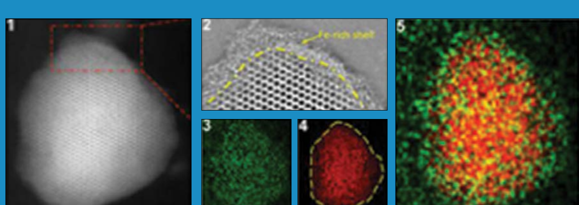
3D reconstruction of lithium-ion battery cathode using FIB-SEM serial sectioning.

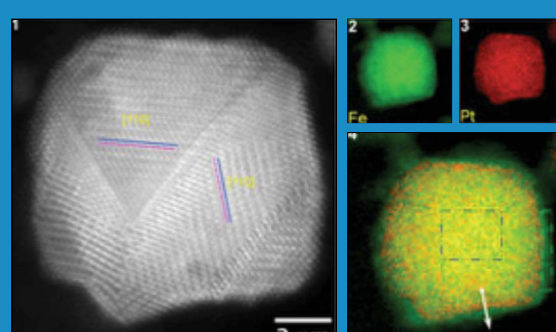
REFERENCES 1) Three-dimensional investigation of cycling-induced microstructural changes in lithium-ion battery cathodes using focused ion beam/scanning electron microscopy. H. Liu, J. M. Foster, A. Gully, S. Krachkovskiy, M. Jiang, Y. Wu, X. yang, B. Protas, G. R. Goward, G. A. Botton, J. Power Sources, 306 (2016), 300.

2) Spatially resolved surface valence gradient and structural transformation of lithium transition metal oxides in lithium-ion batteries. H. Liu, M.Bugnet, M. Z. Tessaro, K. J. Harris, M. J.R. Dunham, M.g Jiang, G. R. Goward, G. A. Botton, Phys. Chem. Chem. Phys., 18 (2016) 29064.

Surface Segregation of Fe in Pt–Fe Alloy Nanoparticles for Electrocatalysis

Electron microscopy with in-situ heating allows the study of phase transformations in single nanoparticles, such as Pt–Fe alloy nanoparticles of potential use in fuel-cell electrocatalysis. The data shows that Fe (instead of Pt) segregates towards the particle surface during annealing. The surface segregation of Fe precedes the disorder-to-order transition and affects the ordered phase evolution dramatically; ordering initiates at the Fe-rich shell. This study indicates the potential for rational design of Pt-Fe nanoparticles through control of their phase evolution, ultimately leading to their improved performance in fuel-cell electrocatalysis.





Atomic-resolution images and composition data for two different Pt–Fe nanoparticles annealed at 800 °C for 1 hour. Fe is shown in green and Pt in red.

REFERENCE Surface Segregation of Fe in Pt–Fe Alloy Nanoparticles: Its Precedence and Effect on the Ordered-Phase Evolution during Thermal Annealing, Sagar Prabhudev, Matthieu Bugnet, Guo-Zhen Zhu, Christina Bock, Gianluigi A. Botton, ChemCatChem 7 (2015) 3655–3664