中央大學物理學系

Department of Physics, National Central University

Colloquium

Probing Nanoscale Electronic and Atomic Structural Evolution in Energy Materials by Synchrotron X-ray Microscopy and Spectroscopy

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Abstract :

Synchrotron-based X-ray techniques provide an effective way to examine the electronic and structural evolution of functional materials over different length scales. Among them, scanning transmission X-ray microscopy (STXM) is particularly useful because it combines element-specific spectroscopy with nanoscale spatial resolution, allowing local chemical and electronic variations within individual particles to be directly observed. Ptychographic imaging can further improve the spatial resolution, while X-ray absorption fine structure (XAFS) provides complementary information on local bonding, coordination, and atomic disorder. In this talk, I will present two examples of how these techniques can be used to study degradation and stabilization mechanisms in layered oxide cathodes for lithium-ion batteries. For charged $LiNi_{0.8}Co_{0.1}Mn_{0.1}O_2$ (NCM811), in situ heating STXM reveals that the thermal degradation pathway strongly depends on the electrolyte environment. In solid electrolytes, Ni reduction and oxygen loss begin from the particle interior and gradually propagate outward. In liquid electrolytes, the degradation instead starts from the surface and moves toward the core. XAFS measurements further show that these changes are accompanied by increasing local disorder around Ni and weakening of the Ni-O framework. The second example concerns lithium- and manganese-rich layered oxides (LMR). STXM resolves clear shell–core differences in electronic structure after surface Al incorporation. The modified surface promotes orbital reconstruction and Ni 3d t2g-O 2p-Mn 3d t2g π-type superexchange interactions, which help suppress excessive oxygen anionic redox and irreversible oxygen release at high voltage. XAFS further confirms changes in Ni-O bonding and local coordination.

These results show how STXM and XAFS can be used together to connect nanoscale electronic heterogeneity with local atomic structure and to better understand the origin of instability in high-energy cathode materials.