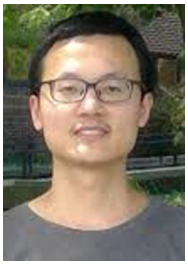
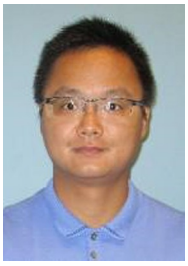
Cover Profile
doi.org/10.1002/batt.202100296

Chemistry Europe
European Chemical Societies Publishing

New Insights into Structural Evolution of $LiNiO_2$ Revealed by Operando Neutron Diffraction


Po-Hsiu Chien


Xianyang Wu


Bohang Song


Zhijie Yang


Crystal Waters


Michelle S. Everett


Feng Lin


Zhijia Du


Jue Liu

OAK RIDGE National Laboratory

VIRGINIA TECH

Invited for this month's cover picture is the group of Jue Liu and co-workers. The front cover shows the operando neutron diffraction study of structural evolution of $LiNiO_2$ cathode in a jelly-type full cell. The anomalous increase of Ni–O bond length at high degrees of charge is successfully captured, bringing new insights into the structure and electronic structure evolution of $LiNiO_2$ at deep charging states. Read the full text of the Article at 10.1002/batt.202100135.

What is the most significant result of this study?

The discovery of the anomalous increase of the average Ni–O bond length in the $LiNiO_2$ at high degree of charge. It is conventionally believed that the H2–H3 phase transition is the intrinsic driving force for the poor cycling performance of $LiNiO_2$. Our discovery highlights that lattice oxygen oxidation (induced anomalous structure change) may also play a critical role.

What was the biggest challenge?

The biggest challenge is the design and commission of the new jelly-roll type in situ cells for operando neutron diffraction.

What new scientific questions/problems does this work raise?

It has been long believed that average Ni–O bond length decreases during charge, but our discovery of the anomalous increase of Ni–O bond lengths at high degrees of charge suggests that the charge compensation mechanism is more complicated in the deeply charged Li_xNiO_2. This may stimulate broad interests in re-visiting the charge-transfer mechanism in late transition metal oxides during oxidation/reduction.