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X-ray absorption spectroscopy and in-operando neutron diffraction studies on local structure fading induced irreversibility in a 18650 cell with P_2-$Na_{2/3}Fe_{1/3}Mn_{2/3}O_2$ cathode in long cycle test

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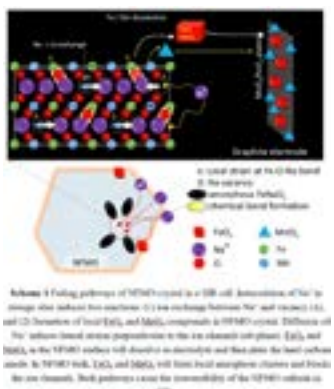
Cathode materials of P_2-$Na_{2/3}[Fe_{1/3}Mn_{2/3}]O_2$ (NFMO) phase nanoparticle with a maximum capacity of ~148 mAh in a sodium ion battery was synthesized by a solid-state annealing method. By cross-referencing results of focused-ion beam (FIB) section scanning electron microscopy, *ex-situ* X-ray absorption spectroscopy (XAS), X-ray photoemission (XPS) depth profiling, and in-operando neutron diffraction, we found that Na ion intercalation and extraction distort the local structure in NFMO crystal, resulting in irreversibility of the sodium ion battery (SIB). This reaction pathway is controlled by the transformation kinetics of the Fe sites from octahedral (Oh) to tetragonal (Td) in the charge and discharge processes. For a SIB operated at 2.0 to 3.8V, steady kinetics between the Na intercalation and chemical state evolution on the Fe sites enable the homogeneous restructuring in both local and global regimes in NFMO crystal. For a SIB operated at 2.0 to 4.5V, substantially higher kinetics in the Fe chemical state evolution induces a dramatic lattice expansion. This expansion cracks the interface between the P_2 and Na intercalated regions, thereby causing substantial irreversibility of NFMO in a SIB.



Recent Publications

1. Sheng Dai, Jyh Pin Chou, Kuan Wen Wang, Yang Yang Hsu, Alice Hu, Xiaoqing Pan, and Tsan Yao Chen (2019) Platinum-trimer decorated cobalt-palladium core-shell nanocatalyst with promising performance for oxygen reduction reaction. Nature Comunication10:440.

2. Yu Zhuang, Jyh Pin Chou, Pang Yu Liu, Tsan Yao Chen, Ji Jung Kai , Alice HU and Hsin Yi Tiffany Chen (2018) Pt3 clusters decorated Co@Pd and Ni@Pd model core-shell catalyst design for oxygen reduction reaction: A DFT study. Journal of Materials Chemistry A 6: 23326-23335.

3. Yu Zhuang, Jyh Pin Chou, Hsin Yi Tiffany Chen, Yang Yang Hsu, Chih Wei Hu, Alice Hu and Tsan Yao Chen (2018) Atomic scale Pt decoration promises oxygen reduction properties of Co@Pd nanocatalysts in alkaline electrolytes for 310k redox cycles. Sustainable Energy Fuels. 2: 946-957.

Biography

Tsan-Yao Chen is currently an Associate Professor at Department of Engineering and System Science, National Tsing Hua University. With more than 10 years of experience in Materials Characterization and 6 years in electronic device (MEMS and IC), failure analysis of multiple executives by Synchrotron Light Source Techniques (at NSRRC, Taiwan). He conduct fundamental materials development in green energy applications including solar cell, fuel cell, and CO2 conversion, water sensing with worldwide collaboration at National rank research team in Russia, USA, Italy, Japan (SPring-8), and UK. He is hosting research projects from academic and industrial funds on physical chemistry researches and environment sensing technologies..

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