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XPS study of redox mechanism in $Na_{2.5-x}Fe_{1.75}(SO_4)_3$ cathode material for high-voltage sodium-ion batteries — •Neama Imam[1], Karsten Henkel[1], Anna Milewska[2], Janina Molenda[2], Ehrenfried Zschech[1], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus-Senftenberg, Germany — [2]AGH University of Krakow, Faculty of Energy and Fuels, Krakow, Poland

A multiplet splitting model based on the original work by Gupta and Sen has been used to track the redox mechanism and electronic structure of $Na_{2.5-x}Fe_{1.75}(SO_4)_3$, a high-performance cathode material for sodium-ion batteries (SIBs). This high-purity, off-stoichiometric open-channel cathode material with a tailored sodium-ion distribution, synthesized using an optimized solid-state route, demonstrates a high operating voltage of ∼3.8 V, surpassing the values reported for other cathode materials in the literature. X-ray photoelectron spectroscopy (XPS) was employed to analyze the evolution of the material's electronic structure at various charging potentials. $Fe2p_{3/2}$ spectra decomposition using the multiplet splitting model revealed the gradual oxidation of Fe^{2+} to Fe^{3+} during battery charging while transitioning from its pristine state ($x = 0$) with the presence of only Fe^{2+} at the cathode surface to the highest sodium de-intercalation level ($x = 1.61$). This result is consistent with the electrochemical analysis.

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