Beyond Conventional Synchrotron-based X-ray Spectroscopy: Fundamental Insights and Application to Positive Electrodes for Metal-ion Batteries

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The design of positive electrode materials for metal-ion batteries has been driven towards the goal of having enhanced safety and achieving high capacity and energy density. These targets mainly rely on the capacity of the electrode material to exchange Li^+ ions (or Na^+ and K^+ ions) quickly and reversibly while operational at larger potential windows. The control of the composition and stoichiometry, as well as the crystal structure, of these electrode materials is a crucial point in design to manifest improved electrochemical properties and higher structural stability. Hence, a holistic understanding of the structure and property relationship is essential.
Various positive electrode materials, including polyanionic compounds and layered transition metal oxides, are investigated using novel characterization techniques utilizing synchrotron radiation sources. This study presents a comprehensive approach to explain the structure-property relationships of the materials by combining structural analysis through X-ray diffraction measurements with hard X-ray spectroscopy studies. Mainly, the project explores the electronic structure of various battery chemistries using beyond conventional X-ray spectroscopic techniques like, high-energy resolution fluorescence-detected X-ray absorption near-edge structure (HERFD-XANES) spectroscopy, non-resonant X-ray emission spectroscopy (XES), and X-ray Raman scattering (XRS).
Specifically, the geometric and electronic distinctions between Tavorite-type $LiVPO_4F$ and KTP-type $KVPO_4F$ are analyzed using HERFD-XANES and XES. Additionally, the ligand and electronic environment in the mixed polyanionic compound $KVPO_4F_{1-x}O_x$ (x = 0, 0.25, 0.5, 0.75, 1) are investigated using valence-to-core XES. Meanwhile, a combination of hard X-ray spectroscopy techniques is employed to probe the strong covalent nature of Ni-O bonds in layered $LiNiO_2$. Finally, both *ex situ* and *operando* X-ray spectroscopy measurements are used to examine the cationic and anionic redox present in Li/Mn-rich layered oxides.
Overall, the application of multiple synchrotron-based X-ray spectroscopy techniques is intended broadly to improve fundamental material understanding and future development strategies.

Jury members :

Mme LYONNARD Sandrine	Directrice de recherche, CNRS-CEA-IRIG	Rapporteure
M. ARČON Iztok	Professor, University of Nova Gorica	Rapporteur
M. STIEVANO Lorenzo	Professeur, Université de Montpellier	Examinateur
M. AYMONIER Cyril	Directeur de recherche, CNRS-ICMCB	Examinateur
M. LONGO Alessandro	Senior Researcher, ISMN-CNR, OUS Palermo	Examinateur
Mme CROGUENNEC Laurence	Directrice de recherche, CNRS-ICMCB	Directrice
Mme IADECOLA Antonella	Ingénieure de recherche, HDR, CNRS-PHENIX	Co-directrice
M. CHOTARD Jean-Noël	Maître de conférences, LRCS-UPJV	Co-encadrant

Vous êtes cordialement invités au pot qui suivra

THÈSE