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Operando X-ray diffraction and absorption spectroscopy to better understand battery materials

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Li-ion and Na-ion batteries operate thanks to reversible intercalation reactions of the intercalant cation (A = Li$^+$ or Na$^+$) with the host compound (A_xH) used as the active material of the positive electrode (often referred as “cathode”). These intercalation reactions typically exhibit two types of reaction mechanisms: (i) homogeneous reactions (single phase or solid solution), which involve the formation of a non-stoichiometric compound whose insertion content x in A_xH continuously varies throughout the intercalation domain $x_{min} \geq x \geq x_{max}$; or (ii) heterogeneous reactions (multi-phase) which involve the nucleation and growth of a second phase A_yH (where $y \neq x$) as a result of the compositional changes occurring within the electrode. In single-phase reactions, the host structure does not suffer from major structural changes other than a continuous variation in volume to accommodate the change in composition, which is generally considered to be more favorable for fast diffusion than the moving interface found in two-phase reactions. On the other hand, depending on the rate at which these intercalant reactions occur (*i.e.* depending on the rate imposed to the battery for the charge and/or discharge processes), the electrodes materials are driven away from the equilibrium conditions, which can provoke significant differences in their reaction mechanism, for example changes on the phase transitions sequences.
In this talk, we will illustrate how operando powder X-ray diffraction (XRD) and absorption spectroscopy (XAS) experiments provide valuable insights for the understanding of the reaction mechanisms in electrode materials such as Li-rich layered oxides [1], the high-voltage spinel $LiNi_{0.5}Mn_{1.5}O_4$ [2] and the Na-ion triphylite (olivine-type) $NaFePO_4$ and $NaFe_{0.8}Mn_{0.2}PO_4$ cathode materials [3,4].

References

1. Benoit Mortemard de Boisse, Marine Reynaud, Atsuo Yamada, et al. Coulombic self-ordering upon charging a large-capacity layered cathode material for rechargeable batteries. *Nature Communications* 2019. DOI: 10.1038/s41467-019-09409-1.
2. Marcus Fehse, Marine Reynaud, *et al.* Influence of Transition-Metal Order on the Reaction Mechanism of LNMO Cathode Spinel: An Operando X-ray Absorption Spectroscopy Study. *Chemistry of Materials* 2022 DOI: 10.1021/acs.chemmater.2c01360.
3. Damien Saurel, Marine Reynaud, Montse Casas-Cabanas, et al. Rate dependence of the reaction mechanism in olivine NaFePO4 Na-ion cathode material. *Int. Journal of Energy Research* 2018. DOI: 10.1002/er.4078.
4. Damien Saurel, Marine Reynaud, Montse Casas-Cabanas, et al. The triphylite $NaFe_{1-y}Mn_yPO_4$ solid solution ($0 \leq y \leq 1$): Kinetic strain accommodation in $Na_xFe_{0.8}Mn_{0.2}PO_4$. *Electrochimica Acta* 2022. DOI: 10.1016/j.electacta.2022.140650.

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