

Using vanadyl sensors to investigate electrolyte degradation in Li-ion batteries

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Li-ion batteries are a key technology for the transition toward a sustainable transportation sector. Successful battery chemistries require a high Faradaic efficiency and long-term stability, which are particularly affected by chemical side-reactions such as electrolyte decomposition and electrode dissolution. The mitigation of detrimental effects caused by reactive trace species necessitates their identification by suitable analytical tools.

For vanadium(+V) oxide cathodes, vanadyl units are released from the electrode upon electrochemical lithium insertion. These endogenously formed ions are exploited as sensors for electrolyte degradation products through complexation. The ligand sphere is determined via EPR hyperfine spectroscopy and compared with DFT calculations. [1]

Depending on the operation/storage condition, spectral characteristics indicate different ligand environments of the vanadyl ion, originating from degradation products of the electrolyte solvent propylene carbonate or electrolyte salt LiPF_6 . Furthermore, structural flexibility manifested in unusual ^{31}P and ^{19}F hyperfine spectroscopy traces was identified, as has been similarly observed for a Cu(II) complex recently. [2]

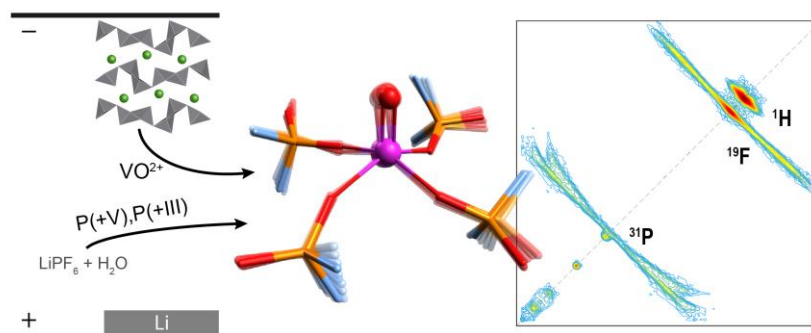


Figure 1: Schematic depiction of the formation of vanadyl ions with ligands originating from electrolyte degradation. Structural flexibility is manifested in HYSCORE traces.

Literature:

- [1] C. Szczuka, P. Jakes, R.-A. Eichel, J. Granwehr, *submitted* 2021.
- [2] N.-A. Stamos, E. Ferentinos, M. Chrysina, C. P. Raptopoulou, V. Psycharis, Y. Sanakis, D. A. Pantazis, P. Kyritsis, G. Mitrikas, *Inorg. Chem.* 2020, 59, 3666–3676.