NMR and EPR characterization of V₂O₅ as a cathode material for high-capacity Li-ion batteries

Conrad Szczuka^{a,b}, Peter Jakes^a, Rüdiger-A. Eichel^{a,b} and Josef Granwehr^{a,c}

^aInstitute of Energy and Climate Research (IEK-9), Forschungszentrum Jülich, Jülich, Germany

^bInstitute of Physical Chemistry, RWTH Aachen University, Aachen, Germany ^cInstitute of Technical and Macromolecular Chemistry, RWTH Aachen University, Aachen, Germany

Li-ion batteries are the key technology for the electrification of the transport sector. Their enhancement requires fundamental understanding of the battery chemistry involving solid-state and interface reactions and processes. NMR and EPR were successfully applied to investigate battery materials in many cases [1,2], however, mostly independent from each other. Here, both techniques are applied to investigate the cathode material V₂O₅. We exploit the strengths of EPR to target dilute surface defects and monitor redox reactions, and the strengths of NMR to identify phase transitions and the local surrounding of the nuclei under investigation.

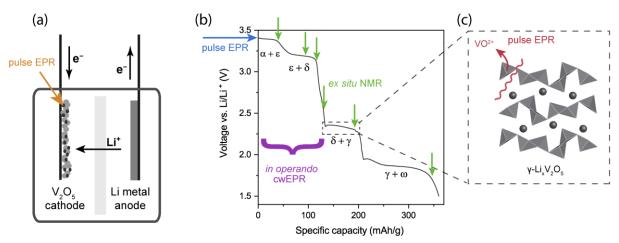


FIGURE 1. Overview of electrochemical testing of V_2O_5 cathodes in Li-ion batteries. Applied magnetic resonance techniques are indicated in color. (a) Schematic of the used battery setup with a V_2O_5 working electrode, a lithium metal counter and reference electrode, and a seperator. EPR-active defects are introduced through cathode film preparation. (b) Electrochemical discharge profile showing voltage plateaus that indicate distinct phase transitions. $\text{Li}_x V_2 O_5$ phases are indicated with greek letters. (c) Upon the δ -> γ phase transition, vanadyl ions are released from the bulk cathode.

Acknowledgements

We thank P. P. M. Schleker and E. Veroutis for initial help with NMR experiments.

References

[1] O. Pecher, J. C.-Gonzalez, K. J. Griffith, C. P. Grey, *Chem. Mater.* **2017**, 29, 213–242.

[2] A. Niemöller, P. Jakes, S. Eurich, A. Paulus, H. Kungl, R.-A. Eichel, J. Granwehr, *J. Chem. Phys.* **2018**, *148*, 014705.