



MAX PLANCK INSTITUTE FOR
SOLID STATE RESEARCH



Special Online Colloquium Series "Future of Electrochemistry"

September 17, 2020 • 2 p.m.

Lithium Transition Metal Oxides What happens when electrons are removed from O^{2-} ?

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Lithium transition metal oxide intercalation compounds are the basis of cathodes in Li-ion batteries. On charging, Li^+ is removed from the lattice with charge compensation by oxidation of the transition metal ion, e.g. Li^+ is extracted from $LiMn_2O_4$ while Mn^{3+} is oxidised to Mn^{4+} . Limiting oxidation to the transition metal limits the capacity to store charge and hence the energy density of the Li-ion battery. For more than 20 years it has been known that more Li^+ can be removed from certain compounds than is charge compensated by Tm oxidation. The archetypal examples are the layers compounds: $Li[Li_{0.2}Ni_{0.2}Mn_{0.6}]O_2$ and $Li[Li_{0.2}Ni_{0.13}Co_{0.13}Mn_{0.54}]O_2$. Understanding the origin of this phenomenon has proved difficult. It is now known that electrons are removed from the O^{2-} ions (holes in the O valance band) but the nature of the hole states, their link to the resulting structural changes and how understanding this might be harnessed to increase the energy storage of Li-ion batteries is only now crystallising.

I shall show, using a range of techniques including XAS, RIXS, STEM, NMR, diffraction and DFT, that across a wide range of alkali metal rich transition metal oxides, O^{2-} is oxidised to O_2 . The O_2 is either evolved from the surface or trapped in voids formed in the bulk by reorganisation of vacancies within the structure. Although O_2 can be reduced back to O^{2-} , the process is not energetically reversible, explaining the much lower voltage on discharge compare with the first charge (approx. 1 eV less), the phenomenon of so-called voltage hysteresis. Furthermore, it is possible to suppress O_2 formation, trapping hole states on O^{2-} and obtaining energetic (voltage) and structural reversibility. Such behaviour points the way to awards high energy density cathodes for Li-ion batteries.

The scientific talk will be broadcasted via **ZOOM**. You will receive the login data by email.

All members of the institute are cordially invited.