New discovery for better batteries

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Materials researchers at Uppsala University have made new discoveries in understanding energy storage in lithium-ion (Li-ion) batteries. This will help in the design of new materials for future batteries with significantly higher storage capacity than up to now.

Working with researchers from the Universities of Oxford and Kent in England and from the USA, researchers from Uppsala University are looking into special kinds of Li-ion battery materials which can provide batteries with higher energy levels those in use today.

'We discovered for the first time that oxygen in the electrodes behaved in an unexpected manner. Usually, oxygen takes up two electrons as fast as it can. In this material, it released one of them again and this is what provides the higher capacity seen in the charging process,' says Laurent Duda, university lecturer in physics at Uppsala University.

The study, published in *Nature Chemistry* on 21 March, was produced by scientists from a number of different fields of research and was carried out using a synchrotron light source called Advanced Light Source, ALS. Advanced X-ray spectroscopy was necessary to understand how the materials work. This is a sophisticated spectroscopic technique which researchers at Uppsala University have helped to develop over the last 25 years since its inception.

Li-ion batteries are well-known power sources found in almost all portable electronics, such as mobile phones, computers and household appliances. Battery development is mainly focused upon producing more

powerful batteries with greater capacity and power output. There are many different kinds of materials which can be used in lithium batteries and they all have different kinds of useful properties.

'It has been mostly oxide materials with a combination of metals such as nickel, cobalt and manganese which have seemed the most promising storage electrodes for high energy in lithium batteries. But certain combinations of metals give an unexpectedly high storage capacity and the reason for this has been argued about for a long time,' says Kristina Edström, professor of chemistry at Uppsala University.

Researchers previously thought that the extra storage capacity depended only upon unwanted side effects which produce oxygen in the electrolyte when lithium batteries are charged to their limit. Another possible explanation has been that so-called peroxides have been formed which break down the electrode material.

For the new study, researchers used advanced X-ray spectroscopy to examine a variant of a so-called Li-rich material. Other methods provide summary information on the battery material but with X-ray spectroscopy it is possible to follow how every kind of atom behaves when a battery is being charged.

According to the study, only some oxygen atoms in the material act this way, namely those close to manganese and lithium, where they form a 'localized island' until the battery is discharged again.

'This discovery will enable us to research into ways to customize materials combinations with appropriate manganese content levels,' says Laurent Duda.

More information: Kun Luo et al. Charge-compensation in 3d-transition-metal-oxide intercalation cathodes through the generation of

localized electron holes on oxygen, *Nature Chemistry* (2016). DOI: 10.1038/nchem.2471