Chemistry Colloquium

Oxygen-redox Chemistry in High Energy Density Battery Cathodes

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Host: Stefan Freunberger

One of the biggest challenges facing lithium-ion batteries is how to increase their energy density. The cathode, typically a layered lithium transition metal oxide, represents a major limitation. One route to increase the energy density is to store charge at high voltage on the oxide ions in the cathode material. However, removing electrons from lattice oxide ions typically results in structural instability leading to voltage hysteresis and voltage fade over cycling. Understanding the mechanism behind oxygen redox is critical to overcoming these issues.Our recent investigations into Li-rich cathodes have revealed that oxidized oxygen takes the form of O2 molecules which are trapped in nanovoids in the structure. We have also shown that these trapped O2 molecules can be reduced back to O2- on discharge providing a viable charge storage mechanism to explain oxygen redox. In this talk, I will discuss the evidence1-3 for the formation and reduction of trapped O2 and explore the impacts this has on the performance of oxygen redox cathodes, such as voltage hysteresis and fade.4,5 I will show how the formation of O2 extends to 4d and 5d transition metal oxides5, disordered rocksalt cathodes6 and even to non-Li-rich cathodes7. Finally, I will show that it is possible to suppress this structural change and undergo reversible, high voltage O-redox without voltage hysteresis8. Altogether, this understanding helps to explain the unusual properties of oxygen redox cathodes and informs how they might be harnessed to boost the energy density of batteries.

Thursday, October 31, 2024 03:30pm - 04:30pm

Moonstone Seminar Room F

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