Superoxide formation in Li₂VO₂F cathode material - A combined computational and experimental investigation of anionic redox activity

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Summary

Anionic redox activity in Li-rich cathode materials is a topic of intense interest because it presents the potential to increase the energy density of Li-ion batteries. An in-depth understanding of the anionic redox activity such as lithiation/voltage levels in which peroxide and superoxide formations take place and the reversibility of the reactions are important. In this work, we present a combined computational and experimental analysis that probes the formation of anionic redox species during electrochemical cycling. We report the formation of peroxides and superoxides in Li₂VO₂F when charged up to a relatively low potential of 4.1 V for Li-rich cathode materials. The formation of superoxide is not entirely reversible upon discharge, which is closely linked to the vanadium dissolution and limited reversibility of the vanadium redox couple. This article provides new insights and fundamental understanding of anionic redox activities in disordered Li-rich materials.

Keywords: Li-rich material; disordered rock salt; anionic redox; superoxide; battery; cathode

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