Anionic redox processes: A transformational approach for advanced energy materials

Redox chemistry provides the fundamental basis for numerous energy-related electrochemical devices, among which Li-ion batteries (LIB) have become the premier energy storage technology for portable electronics and vehicle electrification. Throughout its history, LIB technology has relied on cationic redox reactions as the sole source of energy storage capacity. This is no longer true. In 2013 we demonstrated that Li-driven reversible formation of \((O_2)_n\) peroxo-groups in new layered oxides led to extraordinary increases in energy storage capacity. This finding, which is receiving worldwide attention, represents a transformational approach for creating advanced energy materials for not only energy storage, but also water splitting applications as both involve peroxo species. However, as is often the case with new discoveries, the fundamental science at work needs to be rationalized and understood. Specifically, what are the mechanisms for ion and electron transport in these Li-driven anionic redox reactions?

To address these seminal questions and to widen the spectrum of materials (transition metal and anion) showing anionic redox chemistry, we propose a comprehensive research program that combines experimental and computational methods. The experimental methods include structural and electrochemical analyses (both ex-situ and in-situ), and computational modeling will be based on first-principles DFT for identifying the fundamental processes that enable anionic redox activity. The knowledge gained from these studies, in combination with our expertise in inorganic synthesis, will enable us to design a new generation of Li-ion battery materials that exhibit substantial increases (20 -30%) in energy storage capacity.
storage capacity, with additional impacts on the development of Na-ion batteries and the design of water splitting catalysts, with the feasibility to surpass current water splitting efficiencies via novel (O2)n-based electrocatalysts.

Dziedzina nauki

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