Resource-Friendly and Inexpensive Energy Storage through Engineering of the Electronic Structure and Ionic Transport Properties of Materials

Gerbrand Ceder

Department of Materials Science and Engineering University of California at Berkeley gceder@berkeley.edu

The world is going electric. The growth of electrochemical energy storage is projected to reach several TWh of annual production by 2030, driven by electrification of the automotive market and penetration of electrical energy storage into

the grid. Such rapid growth will strain the supply of Nickel and Cobalt metals used in the layered cathodes oxides of Liion cells. Each TWh of Li-ion energy storage requires almost a million ton of Ni or Co, making growth to multiple TWh extremely challenging. I will discuss how the unique electronic structure of these metals dictates their exceptional performance in Lithium-ion batteries, and how their replacement in current intercalation cathodes will be challenging. Recently developed disordered rocksalt cathodes present a different approach to lithium storage and offer Cobalt and Nickel-free alternative to the layered NMCstyle cathode materials. In these novel materials, welldefined Li transport channels are replaced by statistical percolation of low barrier, Li-rich environments through a cation-disordered landscape. The flexibility of working with a cation-disordered structure creates the option to use a much broader set elements, many of which are abundant and inexpensive. More than a dozen novel cation-disordered cathode materials have been synthesized and tested, most of which contain one or more of either Ti⁴⁺, Nb⁵⁺, Zr⁴⁺, Mo⁶⁺ and a redox-active elements from the group of Mn, Fe, V, Ni.

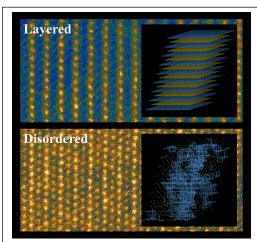


Figure 1: STEM images of typical layered cathode structure (top) and novel disordered rocksalt cathode material (bottom)

While the high-valent cations create short-range order which can destroy Li percolation, we have recently shown that high-entropy systems have reduced short-range order and much high Li transport rates., thereby enabling very high-power cathodes. With DRX cathodes, Li-ion energy storage can reach the holy grail of less than \$100/kWh cost and thereby satisfy most storage needs for grid and transportation.

References

- 1. J. Lee, A. Urban, X. Li, D. Su, G. Hautier, G. Ceder, *Unlocking the Potential of Cation-Disordered Oxides for Rechargeable Lithium Batteries*, Science, 343, 6170, 519-522, DOI: 10.1126/science.1246432 (2014).
- 2. R.J. Clement, Z. Lun, G. Ceder, *Cation-disordered rocksalt transition metal oxides and oxyfluorides for high energy lithium-ion cathodes*, Energy Environ. Sci., 2020,13, 345-373, DOI: 10.1039/C9EE02803J (2020)