Understanding the Voltage in LIB’s

Higher energy density  
Lower cost

Two ways to increase energy density:
1. Increase the amount of lithium that a cathode can insert/remove
2. Increase the voltage

Cell voltage is a measure of the position of the M^{2+/3+} redox couple to that of the Li/Li^+ couple

We investigated the four polyanion cathodes to learn how the crystal structure affects the voltage

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- Electronegativity of counter cation is usually used to determine covalency of the polyanion.
- New generation of polyanion cathodes have same counter cations but different voltages.
- Provided new ways to determine covalency of the polyanion by using hybridization and resonant forms.
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More covalent $X_nO_m$ structure

Increasing electron delocalization

- Polyhedron within the structure can share corners, edges, faces or a combination
- Each type of “sharing” either increases or decreases the electrostatic potential which in turn affects the voltage