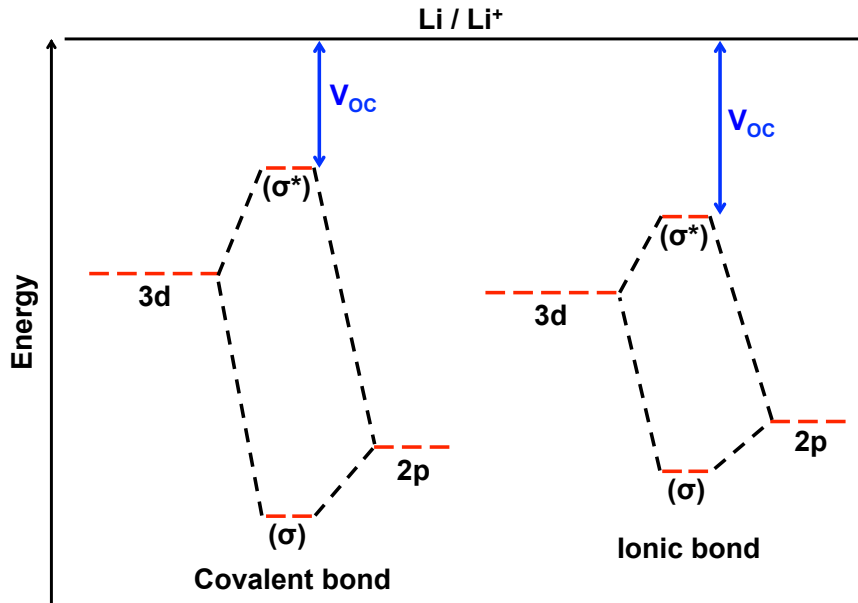


# Understanding the Voltage in LIB's



Higher energy density



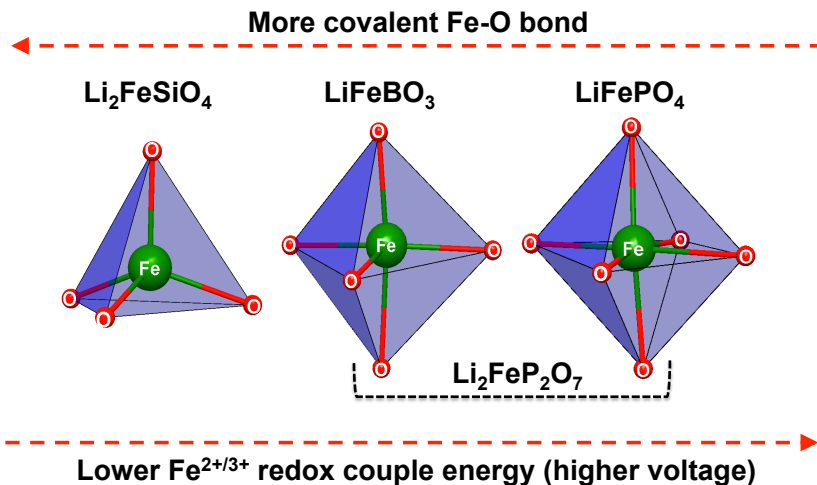
Lower cost

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

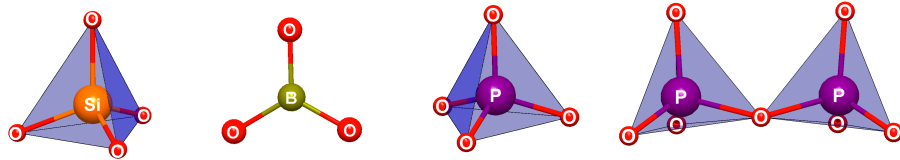
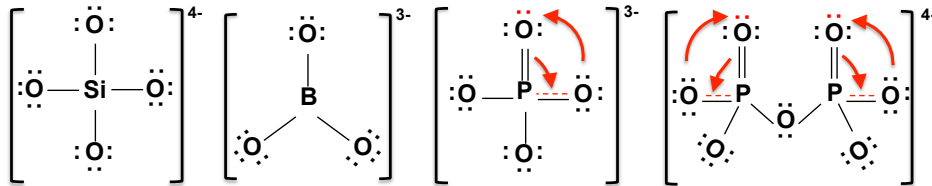
We investigated the four polyanion cathodes to learn how the crystal structure affects the voltage



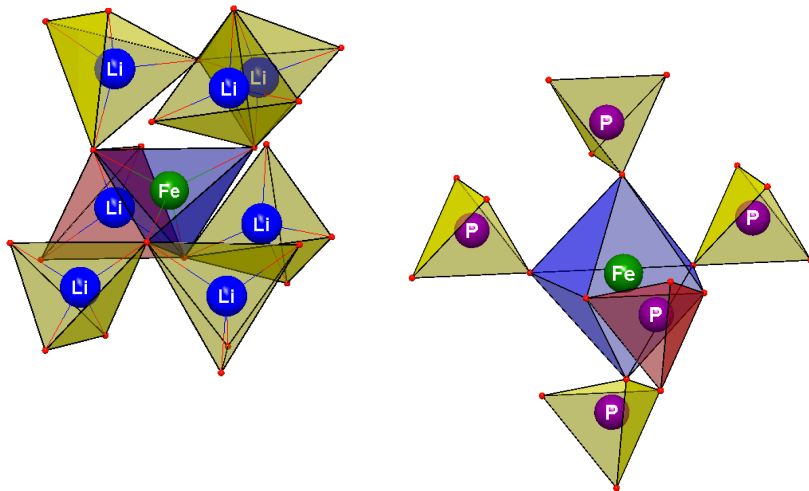
**Ph.D. candidate: Arturo Gutierrez**  
**Advisor: Arumugam Manthiram**

# Understanding the Voltage in LIB's

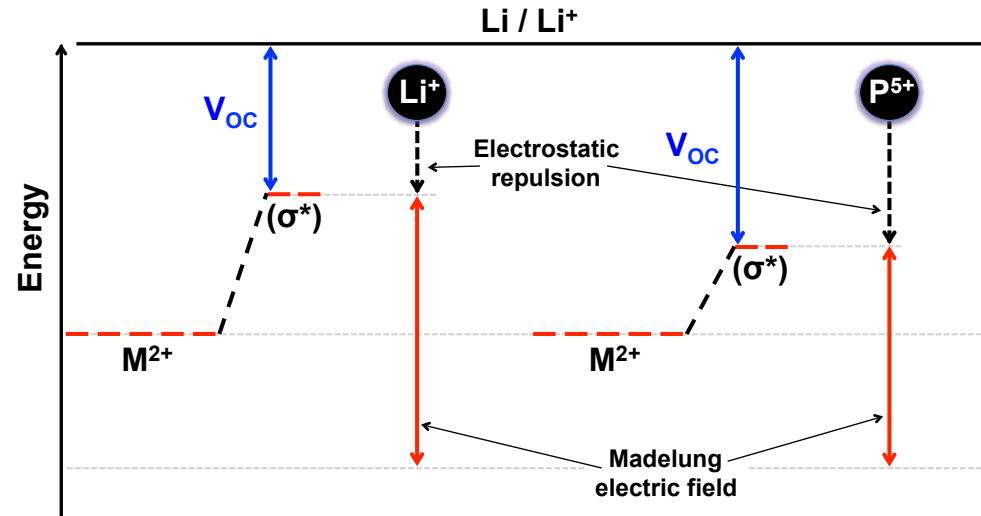
Increasing electron delocalization



More covalent  $X_nO_m$  structure

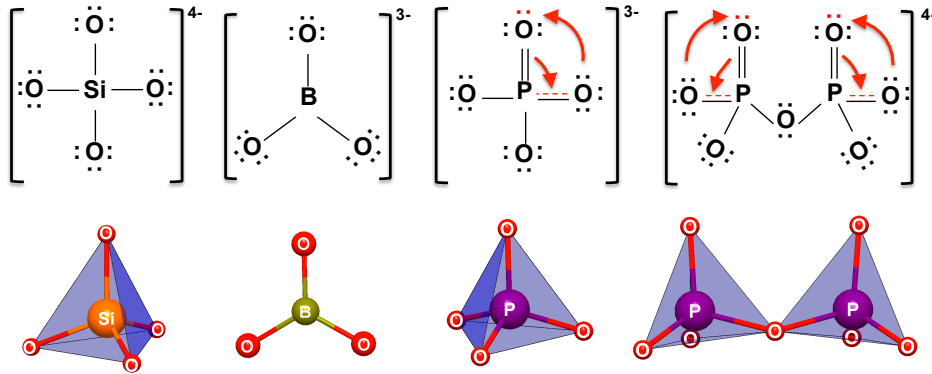


- Electronegativity of counter cation is usually used to determine covalency of the polyanion
- New generation of polyanion cathodes have same counter cations but different voltages
- Provided new ways to determine covalency of the polyanion by using hybridization and resonant forms



# Understanding the Voltage in LIB's

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

More covalent  $X_nO_m$  structure

