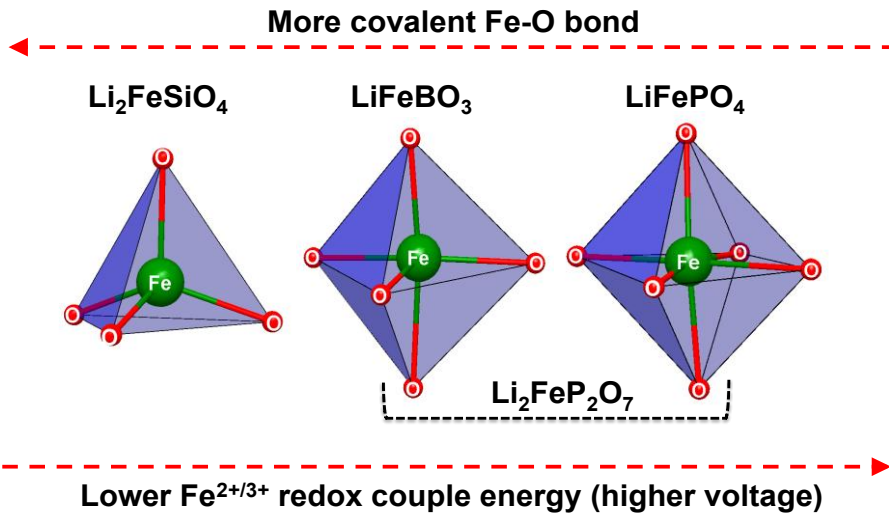
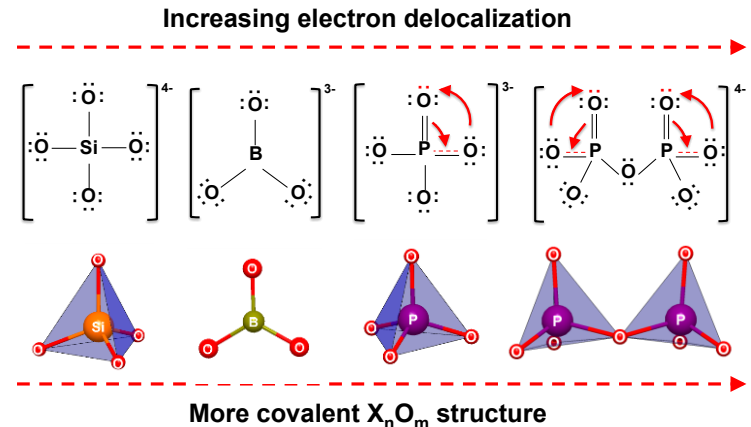


On “tuning” the voltage in LIB’s

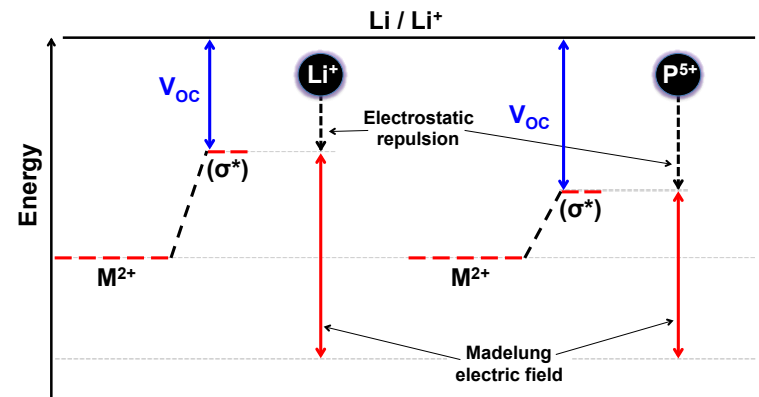
Lithium-ion batteries (LIB’s) are being intensely pursued as energy storage devices because they provide higher energy and power density compared to other systems such as lead-acid and nickel metal-hydride batteries. The energy density of a battery can be increased by using materials that deliver a higher discharge potential. We studied several polyanion cathode systems with the purpose of establishing trends for how structural features affect the discharge potential.



The position of the M^{2+/3+} redox energy is higher when the M-O bond is more covalent. The covalency of the M-O bond increases as the coordination decreases.



The location of the M^{2+/3+} redox couple can be tuned through the inductive effect by “tuning” the covalency of the polyanion.



The strength of the electric field felt by M and produced by other cations can shift the position of the redox energy and either increase or decrease the voltage.