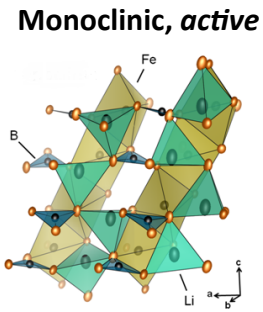
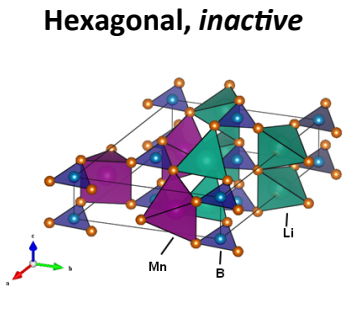
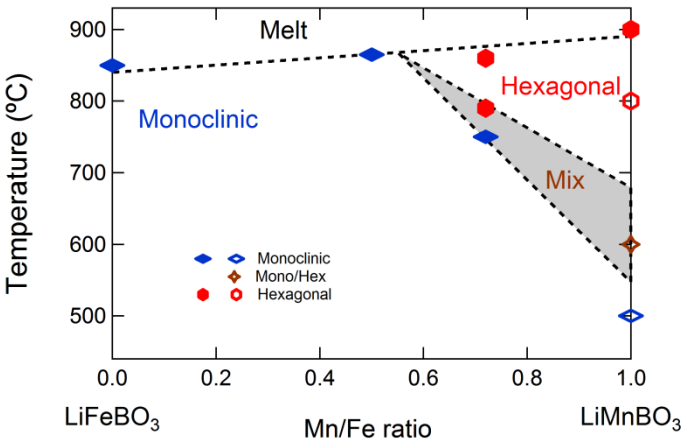
Phase stability of $Li(Fe_{1-x}Mn_x)BO_3$ battery materials







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Scientific Achievement

In situ **determination of temperatures of melting and phase change in the $Li(Mn/Fe)BO_3$ class of emerging high-capacity (220 mAh/g) Li-ion battery cathode materials.**

Significance and Impact

The energy density of high-capacity cathode monoclinic $LiFeBO_3$ can be improved by substituting Mn for Fe, increasing the operating voltage. However, the introduction of Mn also stabilizes a competing hexagonal crystal structure which is electrochemically inactive. This work establishes the stability regimes of both phases under near-equilibrium (*in situ*) conditions.

Research Details

Neutron powder diffraction (HB-2A, HFIR, ORNL) was used to determine high-temperature (300 – 1200 K) crystal structures before, during, and after melting. This information was used to construct a phase diagram for the system, providing insights into optimal synthesis procedures and temperatures for the production of both powder and single crystal samples.