Improving battery performance will be driven by:

- New materials
  - Understanding how the systems function and why they fail
  - New characterization (diagnostics) methods will play a key role
  - Theory development to predict battery function is critical for materials improvement and discovery

Thrust 1: Intercalation Chemistry

LiFePO4 is a good candidate for electrodes with fast rate and good capacity retention. One of the main issues is Fe3+ oxidation, which is realized by XRD and NMR. We have discovered methods to improve the performance.

Thrust 2: Conversion Chemistry

The electrode reaction and delithiation involve electrochemical processes via multi-phase or solid-solution pathways which can be differentiated by the implementation of synchrotron X-ray absorption and scattering spectroscopies (XANES, EXAFS, and PDF).

Thrust 3: Diagnostics

We have designed and fabricated a novel theoretical model for delithiation of LiFePO4, explaining why it can be seen that high rate material despite its first order phase transformation - so small overpotential leads to a solid-solution transformation path. We have also successfully explained the particle size dependence of the lithium diffusion constant in LiFePO4.

Thrust 4: Theory and Modeling

We have developed a novel theoretical model for delithiation of LiFePO4, explaining why it can be seen that high rate material despite its first order phase transformation - so small overpotential leads to a solid-solution transformation path. We have also successfully explained the particle size dependence of the lithium diffusion constant in LiFePO4.

Mission: Provide major fundamental breakthroughs to address future electrical energy storage technology requirements and enable a paradigm shift in energy generation and use

Goal: Identify the key fundamental mechanisms by which electrode materials for rechargeable batteries operate, and the factors that control the rate and the reversibility of these processes

We have focused on new materials discovery based on the success story of LiFePO4:
- Fast rate performance
  - Li moving along one dimension
- Good capacity retention
  - Structure stabilized by strong covalence of oxocations: PO4^3-.