insight into realizing the full 2 Li^+ capacity of multi-electron Li_xVOPO_4

Scientific Achievement

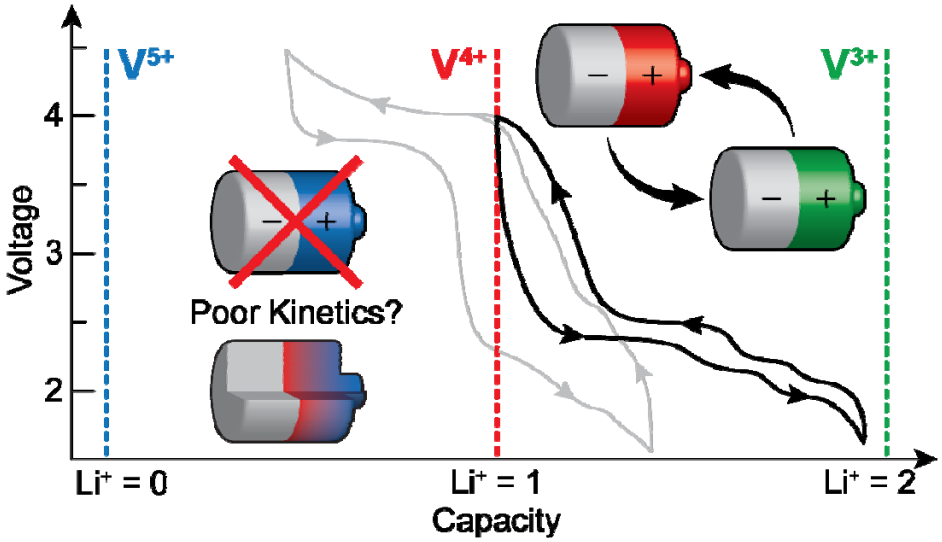
Correlated *full* theoretical capacity (and intermediate phase formation) with *uniform* insertion and extraction of the second Li^+ in solid state synthesized ε-Li_xVOPO_4, a promising multi-electron lithium ion battery (LIB) cathode, by depth-profiling the the low voltage region.

Significance and Impact

Isolated disrupted kinetics in the high voltage reaction as the major hurdle in realizing its full 2 Li^+ capacity.

Research Details

- Used a combination of soft and hard x-ray spectroscopy techniques, both *ex-situ* and *operando*, to depth profile the vanadium redox within the low voltage window.
- Confirmed the predicted intermediate phases, Li_xVOPO_4 (x =1.5 and 1.75) from density functional theory using x-ray spectroscopy.



Findings: Our *ex-situ* **and** *operando* depth-profile studies combining soft **and** hard absorption / photoelectron spectroscopy techniques confirmed full and homogenous second Li^+ insertion and extraction between ε-$LiVOPO_4$ and ε-Li_2VOPO_4 in the low voltage regime. These studies isolated the origin of the Li-ion gradient and capacity loss observed in ε-Li_xVOPO_4 (x = 0 - 2) as originating solely from disrupted kinetics in the high voltage regime. One can cycle between ε-$LiVOPO_4$ and ε-Li_2VOPO_4 without significant capacity loss.

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