

Understanding Li_xFePO_4 Kinetics: From Bulk, to Single Particle, to Many Particles

Scientific Achievement

We have shown through theory and modeling, supported by thorough comparison with the experimental literature, how the kinetics of Li insertion and deinsertion are modified from the bulk, to single-particle, to many-particle scales. We find that single particles transform through a non-equilibrium single-phase mechanism, but particles within an electrode do not necessarily transform in parallel. The multi-particle transport path is found to heavily depend on charging and discharging parameters and cell construction.

Significance and Impact

LiFePO_4 has proven to be effective as a safe and extraordinarily high-rate battery material, yet it only functions as such under specific conditions (in nano-sized particles and in certain cell architectures). Understanding these mechanisms informs the design of better performing batteries.

Research Details

A combination of first-principles calculations and continuum phase-field models were used to characterize the single-particle Li insertion and deinsertion path as well as the interactions *between* particles during the charging and discharging process.

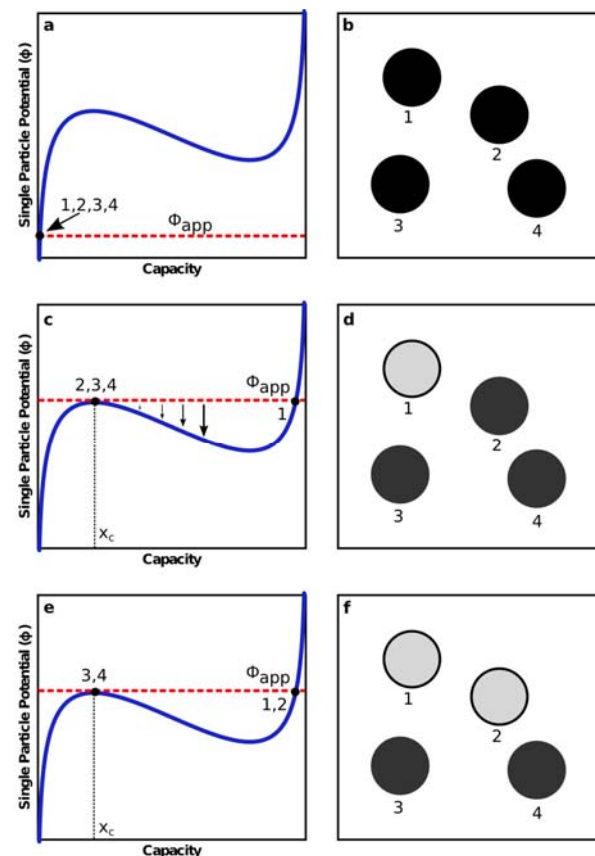


Illustration of how a non-monotonic single-particle potential results in particle-by-particle (dis)charging

R. Malik, A. Abdellahi, G. Ceder – J. Electrochem Soc, 2013, 160(5), A3179–A3197. doi:10.1149/2.029305jes

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