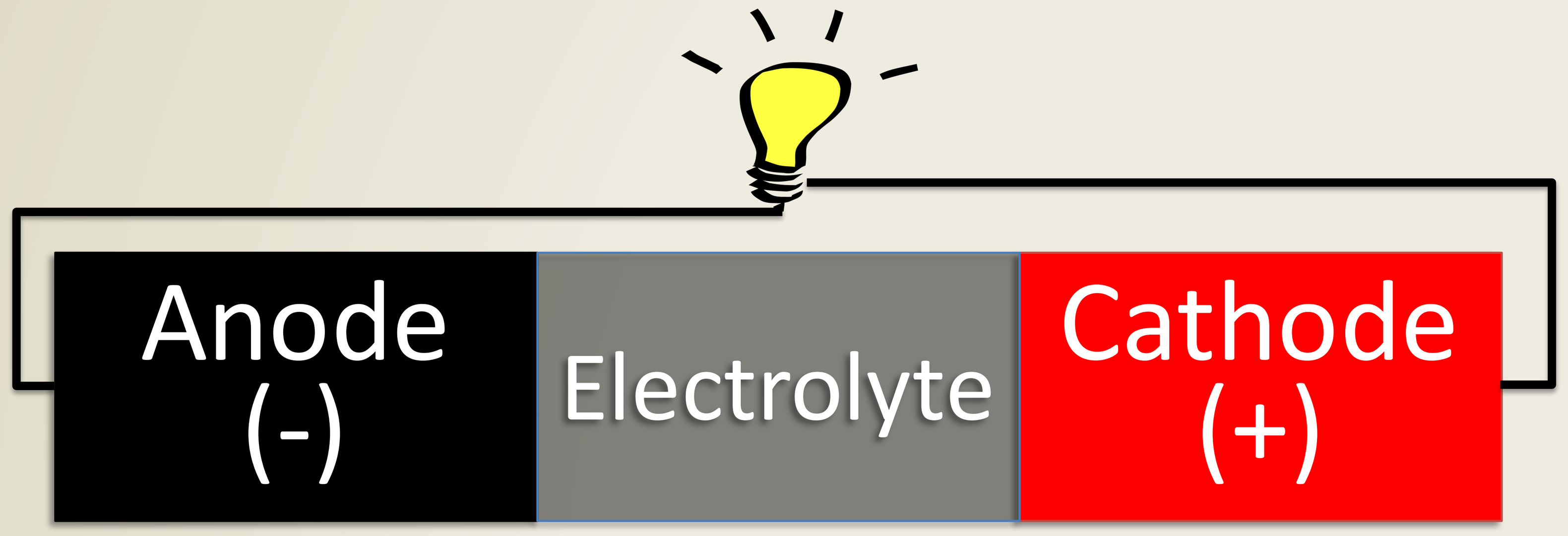
Improving Lithium Ion Battery Technologies with "3-D" Anode Materials

UW Clean Energy Institute

Anatomy of a battery:



Lithium (Li) batteries are powered by the Li oxidation reaction:

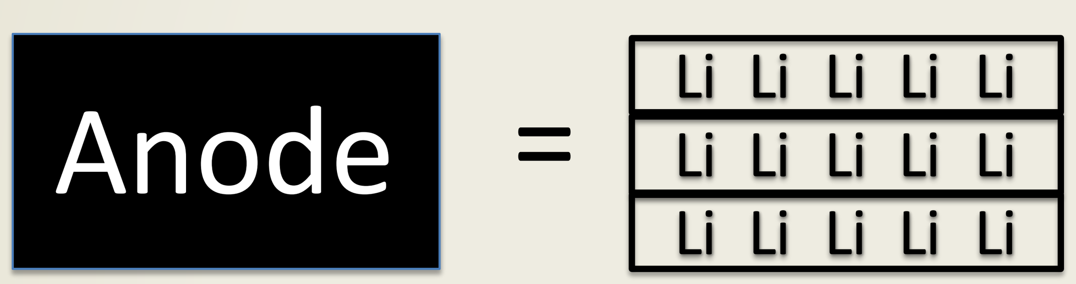
$$\text{Li} \rightarrow \text{Li}^{+} + e^{-} (E_0 = 3.05V)$$

The oxidation potential (E_0) pushes electrons (e^-) generated at the anode through external circuitry, delivering energy to electrical devices ( )

Solid Li anodes give the highest battery capacities:

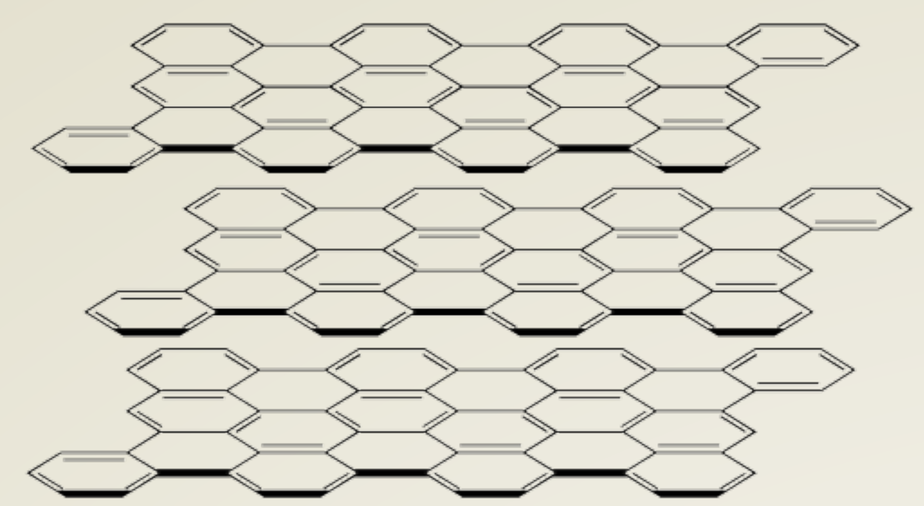
Anode = $\text{Li}_{(s)}$

For rechargablility and safety, the Li must be dispersed in a "cage" material:



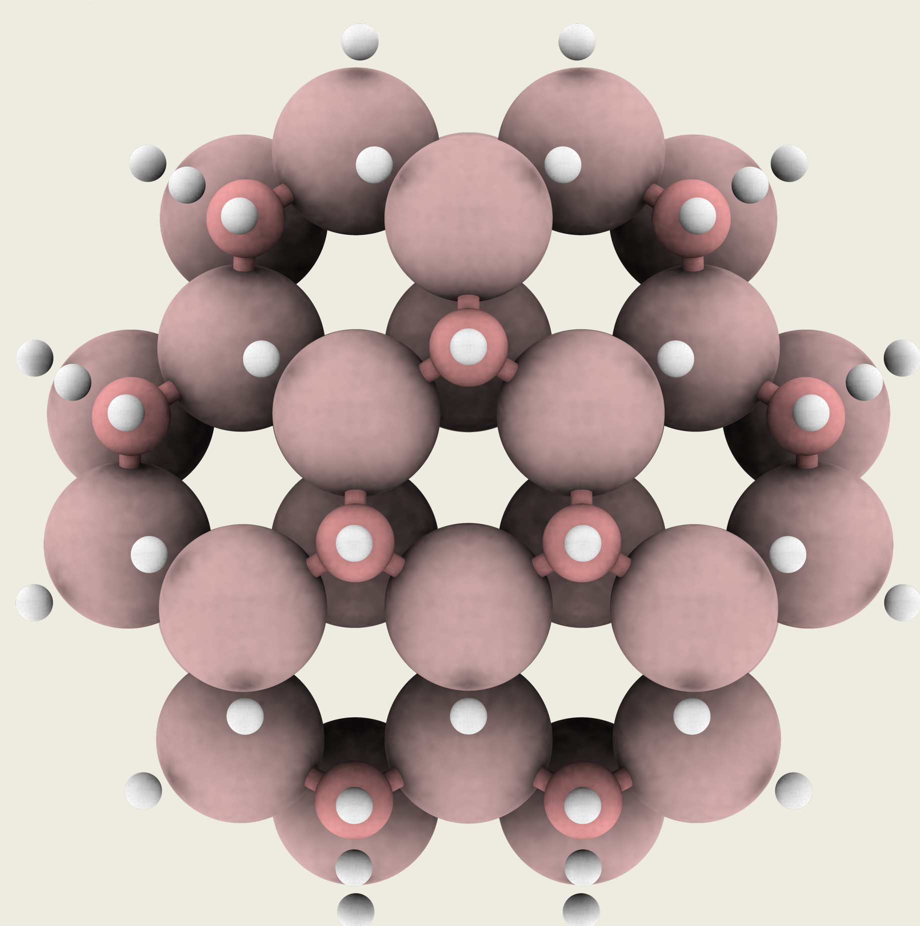
★ Anode materials can be optimized to increase battery life and charge/discharge rates ★

The Li cage material most commonly used in battery anodes as of 2015 is graphite:



Li is stored between sheets of this stacked, 2 dimensional ("2-D") material.

Li packs more space-efficiently in between atoms of some 3-D, crystalline materials (silicon, zinc oxide, etc.):



Research Fellows of the UW Clean Energy Institute are applying the tools of theoretical and computational chemistry to tackle two fundamental challenges in enabling the transition from 2-D to 3-D Li cage materials:

- 3-D cage materials in Li ion battery anodes are degraded by mechanical stress during expansion & contraction while charging & discharging. **The role of crystal impurities in improving cohesion under mechanical stress is being investigated.**

- The diffusion of Li^+ into and out of 3-D materials is not yet well understood. **Li^+ diffusion processes are being simulated via time dependent quantum mechanical methods to establish trends between the lattice structure of emerging 3-D Li cage materials and the Li^+ diffusion pathways & rates they permit.**