Introduction to the Materials Science of

Rechargeable Batteries

Week 1: Basic Concepts, Fundamentals, and Definitions

Lecture 1.2: Charge Figures of Merit in a Battery

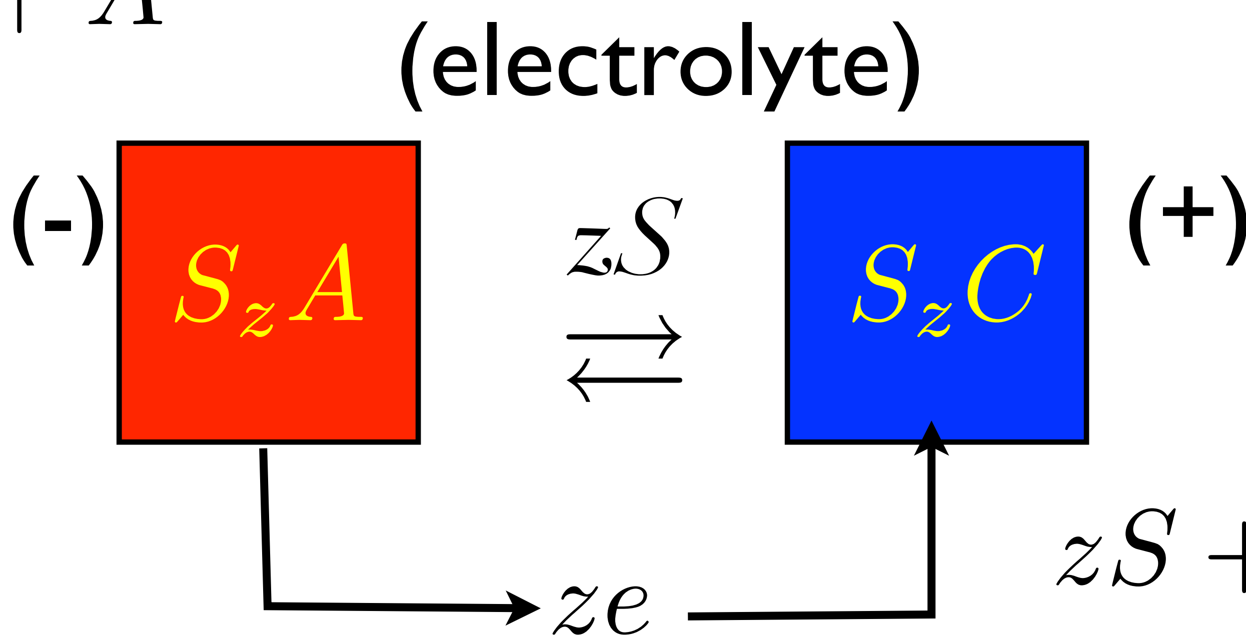
By R. Edwin Garcia
Associate Professor of Materials Engineering
Purdue University

Charge in a Battery

$$S_z A \rightleftarrows zS^+ + A + ze^-$$

C_T^A : anode solubility limit

$$S_z A \rightleftarrows zS + A$$



$$zS + C \rightleftarrows S_z C$$

$$zS^+ + C + ze^- \rightleftarrows S_z C$$

C_T^C : cathode solubility limit

Battery Charge

For Each Phase

$$Q = z \times C_T \times V \times eN_a$$

electronic charge

Avogadro's Number

valence

solubility limit

volume of electrode

$$F = eN_a$$

Faraday's constant

For the Device

$$Q = A \int_{t_\circ}^{t_f} I dt$$

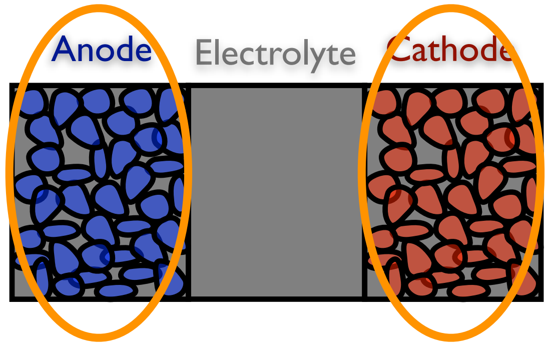
Units:

mA h

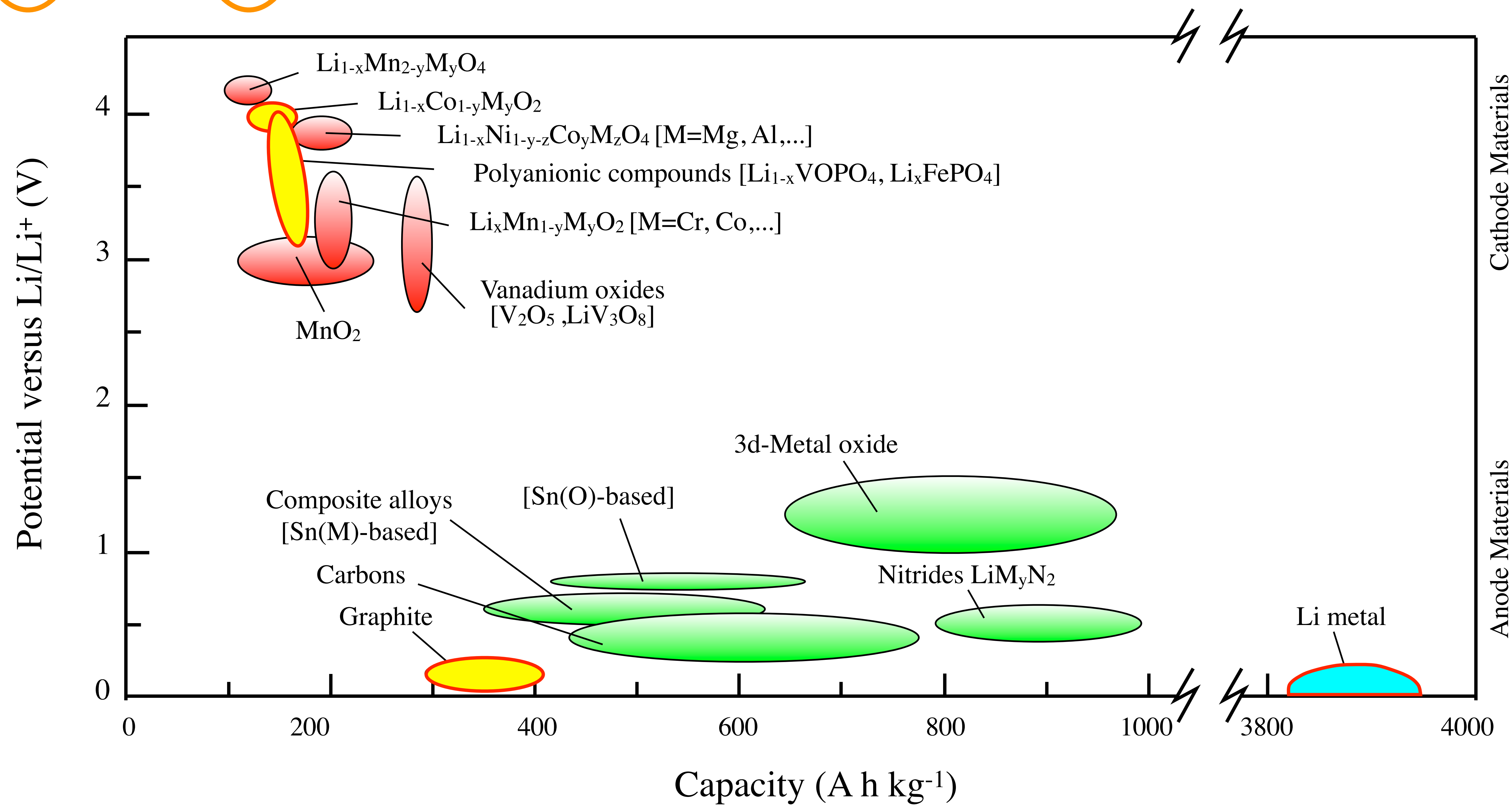
Wish List

- Charge in both electrodes should be balanced, $zFC_T^C \sim zFC_T^A$
- I want $C_T^{C,A}$ to be as large as possible
- Voltage difference should be as large as possible, $\square\varphi_C \gg \varphi_A$
- Rough Figure of Merit:

$$E \sim \varphi_C \times zFC_T^C$$

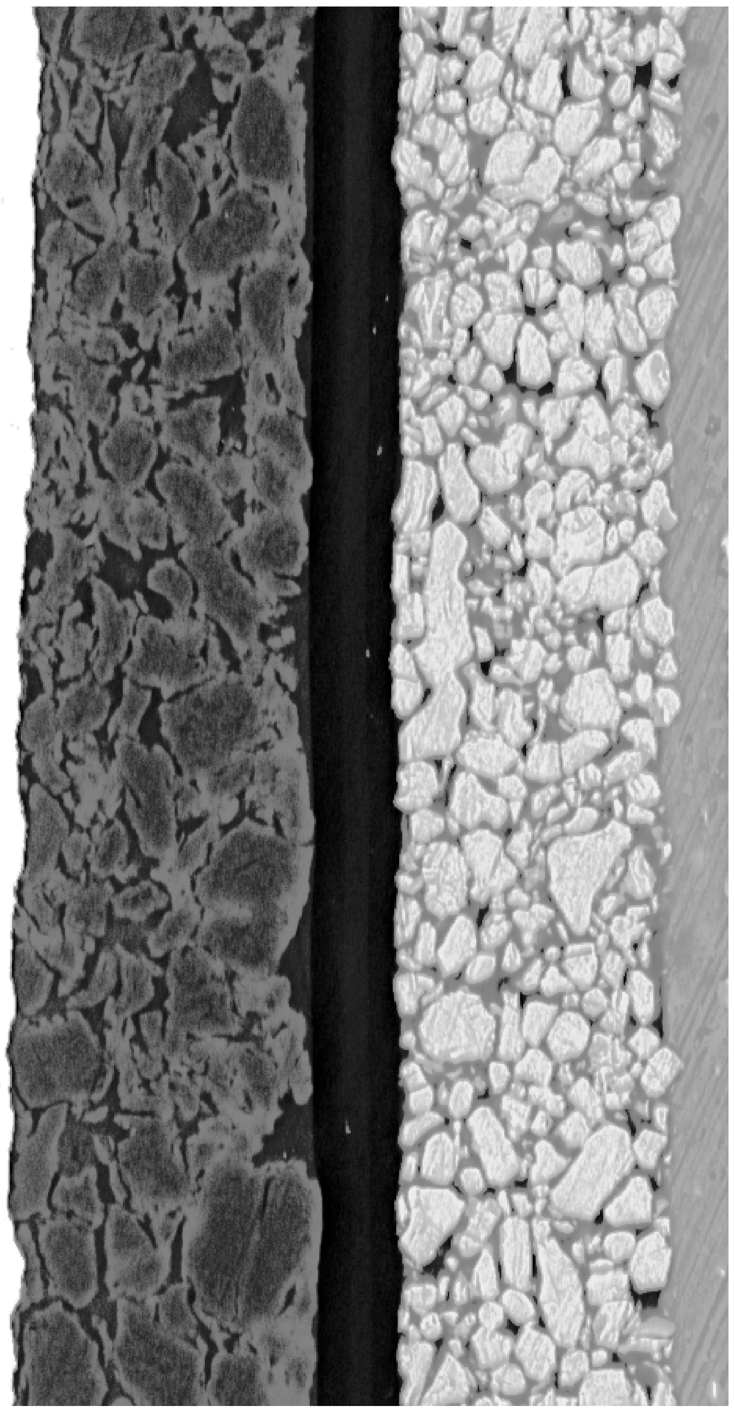


Electrode Materials



J. M. Tarascon and M. Armand. Issues and Challenges Facing Rechargeable Lithium Batteries. Nature, 414:359-367, 2001

Porosity in a Battery

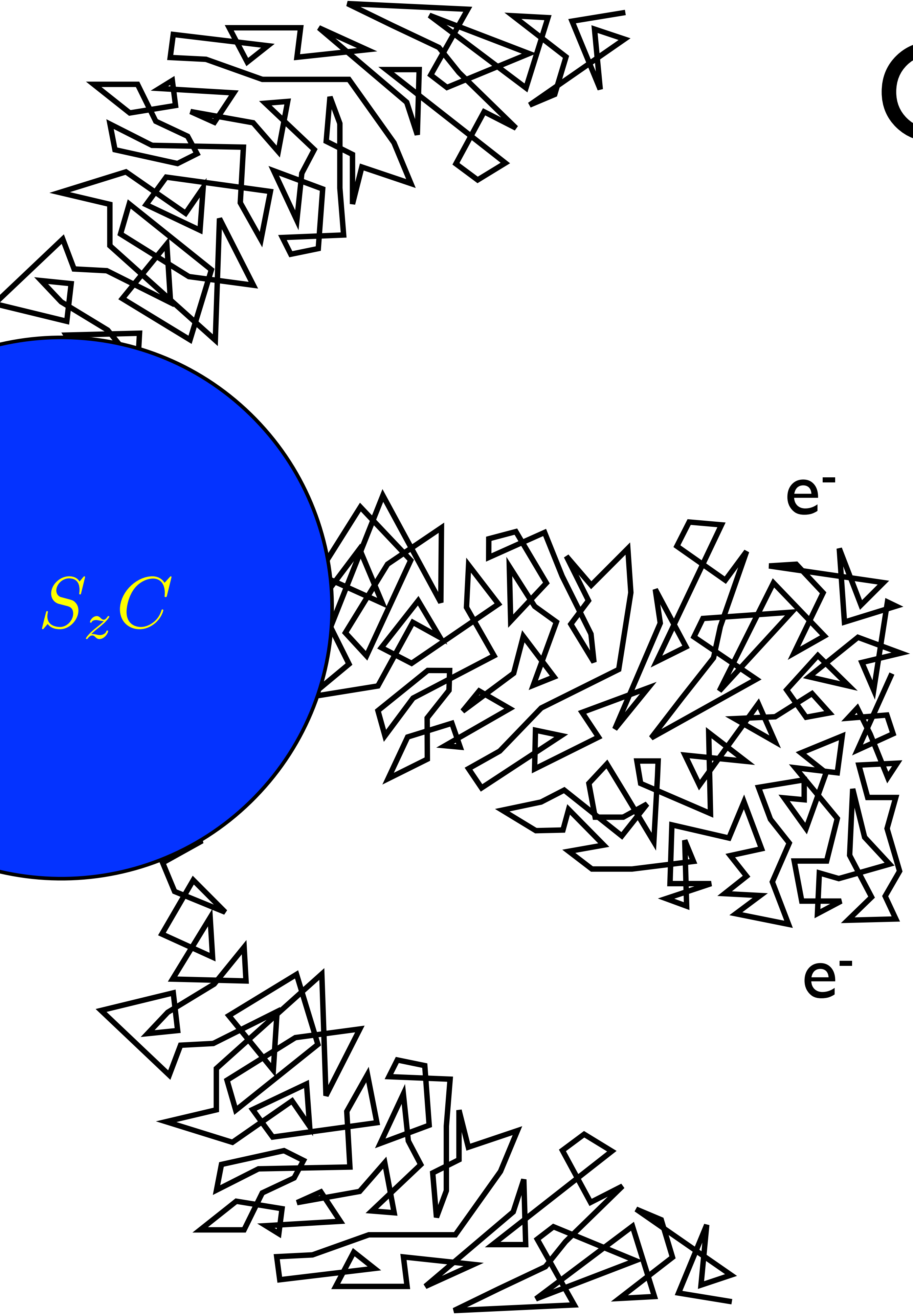


- Made porous to increase reactivity per unit volume of material
- Porosity adds additional transport paths to deliver charge faster
- Porosity is defined as volume fraction left by the active material

$$0 < \epsilon < 1$$

$$Q = z \times C_T \times V \times eN_a\,?$$

Other Porosity Contributions



- Ions and electrons need two routes to flow to the battery particle: need conductive carbon porosity

- Binders and fillers will occupy additional space in the electrode and will impact the capacity and energy density of cell

Porous Battery Capacity

$$V = A \times h$$

For the Entire Device:

$$Q_c = zFc_T^c(1 - \epsilon_c - \epsilon_f)h_c$$

$$Q_a = zFc_T^a(1 - \epsilon_a - \epsilon_f)h_a$$

Units: mA h/m^2

Capacity Ratio

$$R_c = \frac{Q_c}{Q_a} = \frac{c_T^c(1 - \epsilon_c - \epsilon_f)h_c}{c_T^a(1 - \epsilon_a - \epsilon_f)h_a}$$

Units: dimensionless