

# Class Webpage

The screenshot shows a web browser window with the URL [https://nanohub.org/groups/mse597rb\\_2013/wiki/MainPage](https://nanohub.org/groups/mse597rb_2013/wiki/MainPage). The page header includes the nanoHUB.org logo and navigation links. The main content area displays the course title, a 'Main Page' section by R. Edwin Garcia, and a list of resources including a PDF syllabus, lectures, homework, and handouts. A sidebar on the left provides navigation options for the group.

nanoHUB.org  
ONLINE SIMULATION AND MORE FOR NANOTECHNOLOGY

0 New Messages  
R. Edwin Garcia (redwing) Logout My Account

Home Resources Members Explore nanoHUB-U Partners About Support

Home > Groups > MSE 597 Introduction to the Materials Science of Rechargeable Batteries > Wiki > Main Page

MSE 597 Introduction to the Materials Science of Rechargeable Batteries Wiki [New page](#)

**Main Page**  
by R. Edwin Garcia

Article Edit Comments History Delete Index Main Page

Electrochemical materials and its application to energy storage devices, such as batteries and fuel cells are a rapidly growing field, particularly for portable technologies and electric and hybrid vehicles. This course will deliver an introduction to basic electrochemistry, principles of electrochemical devices, electroactive materials used in such systems, and case studies of rechargeable batteries. Theoretical and practical aspects of battery fabrication will be delivered, while placing an emphasis on the integration of electrochemical principles and materials science for rechargeable battery technology. Current trends and directions of the field of battery technology will also be outlined.

[597rbsyllabuscirculation.pdf](#) (165.41 Kb, uploaded by R. Edwin Garcia 11 seconds)

[Lectures](#)

[Homework](#)

[Handouts](#)

Group Manager

Overview

Members 1

Wiki 4

Resources

Discussion

Blog

Wish List

Usage

Projects

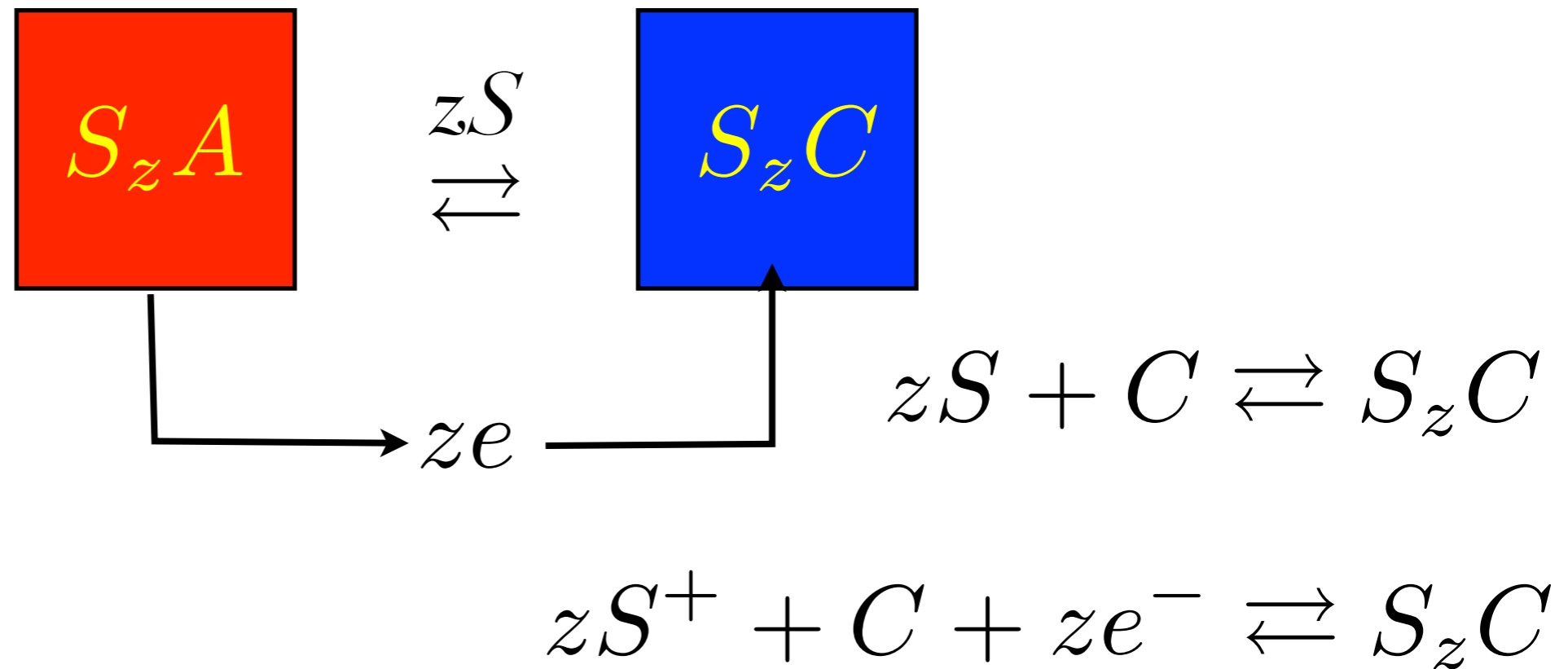
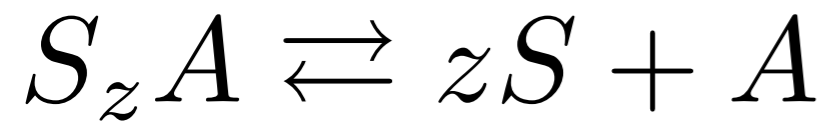
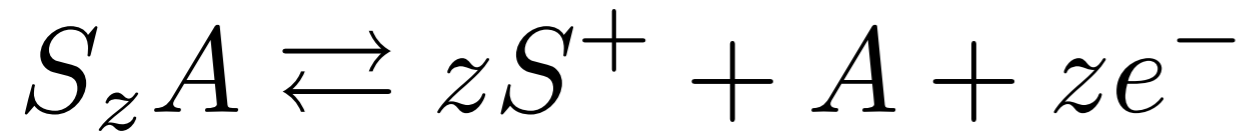
[https://nanohub.org/groups/mse597rb\\_2013/](https://nanohub.org/groups/mse597rb_2013/)

# Groundwork and Basic Definitions I

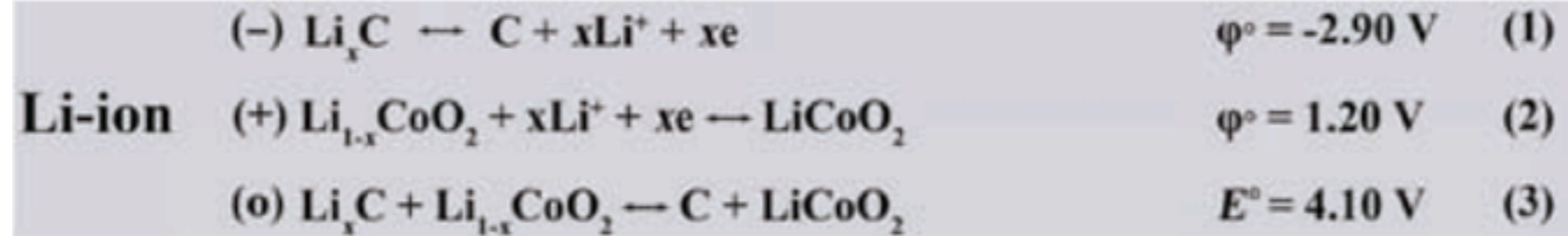
Lectures 2 - 4

R. Edwin García  
redwing@purdue.edu

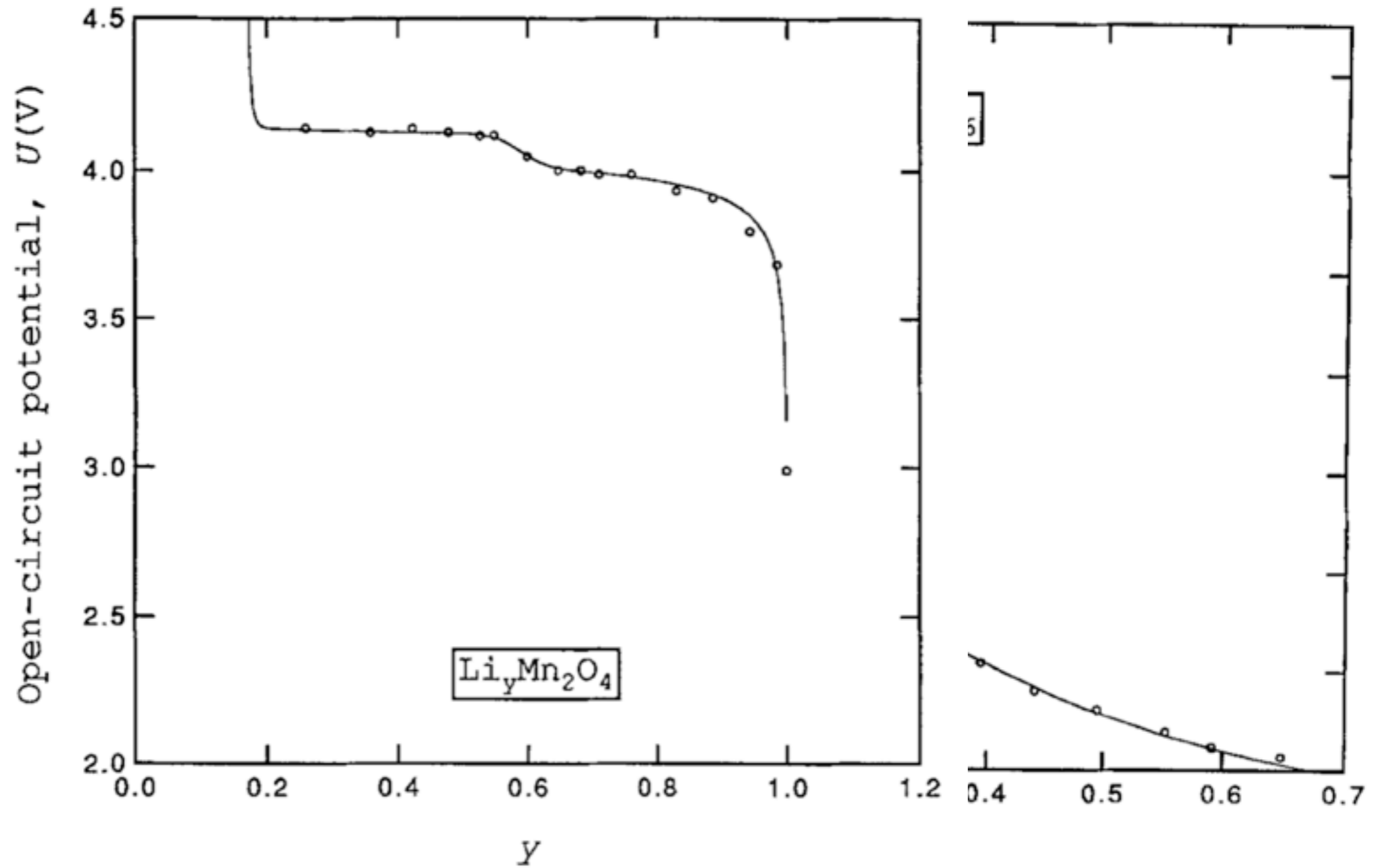
# A Sketch of a Rechargeable Battery



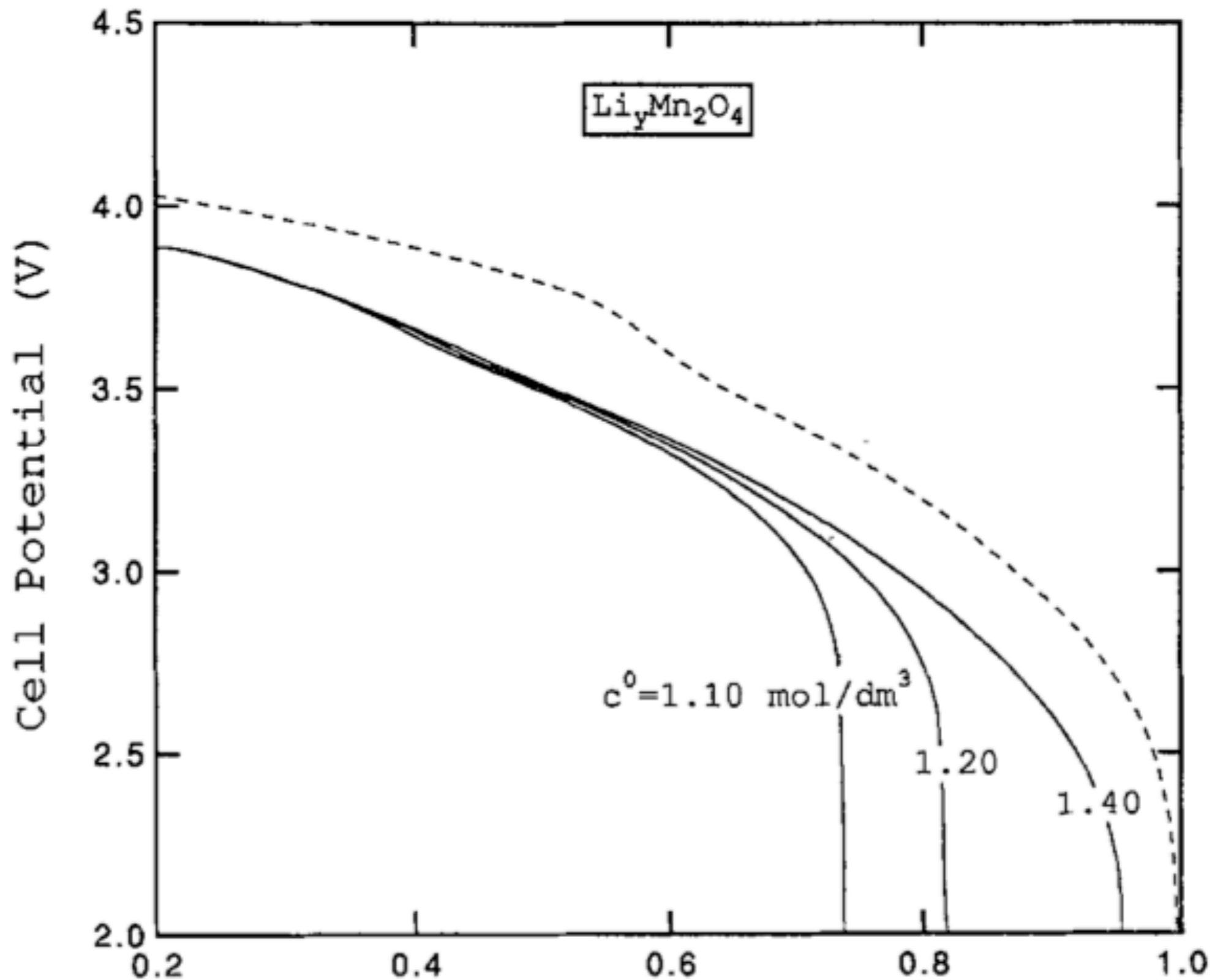
# Example Reactions



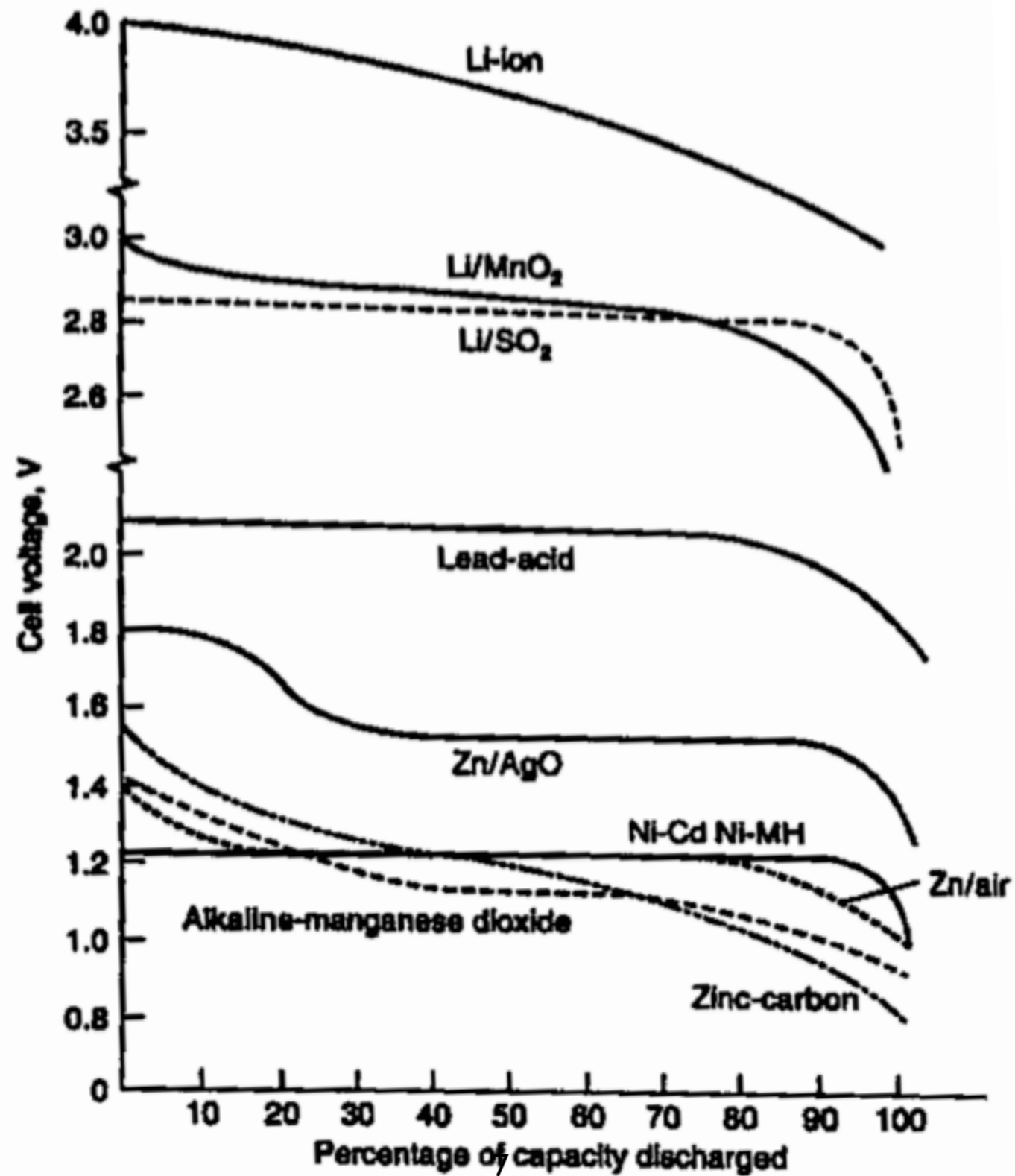
# Battery Voltage



# Capacity Curve



# Battery Voltage



# Battery Charge

For Each Phase

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

valence

solubility  
limit

volume of  
electrode

electronic charge

Avogadro's Number

$$F = eN_a$$

Faraday's constant

For the Device

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

Units:

mA h



# Battery Capacity

For the Entire Device

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

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

Units:

mA h/m<sup>2</sup>

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



# Maximum Theoretical Specific Energy

(MTSE)

For an electrode phase

$$MTSE = \frac{xzFE}{W_t}$$

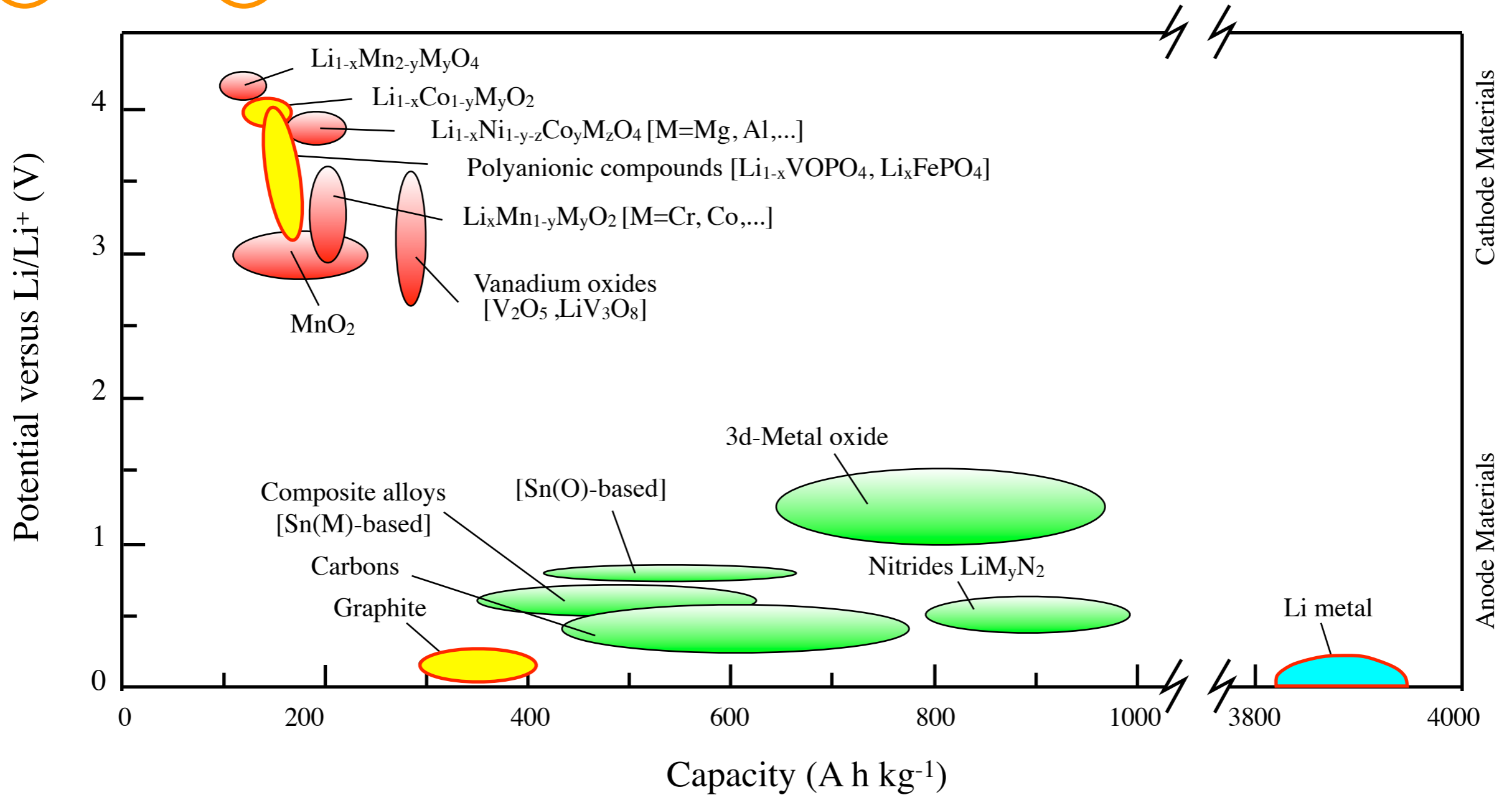
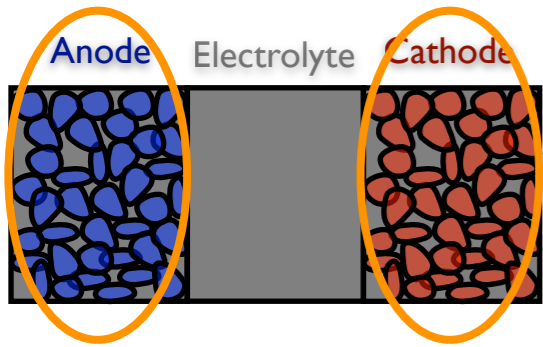
For an entire battery

$$MTSE_B = \frac{\min\{Q_c, Q_a\}(E_c - E_a)}{M_{tot}}$$

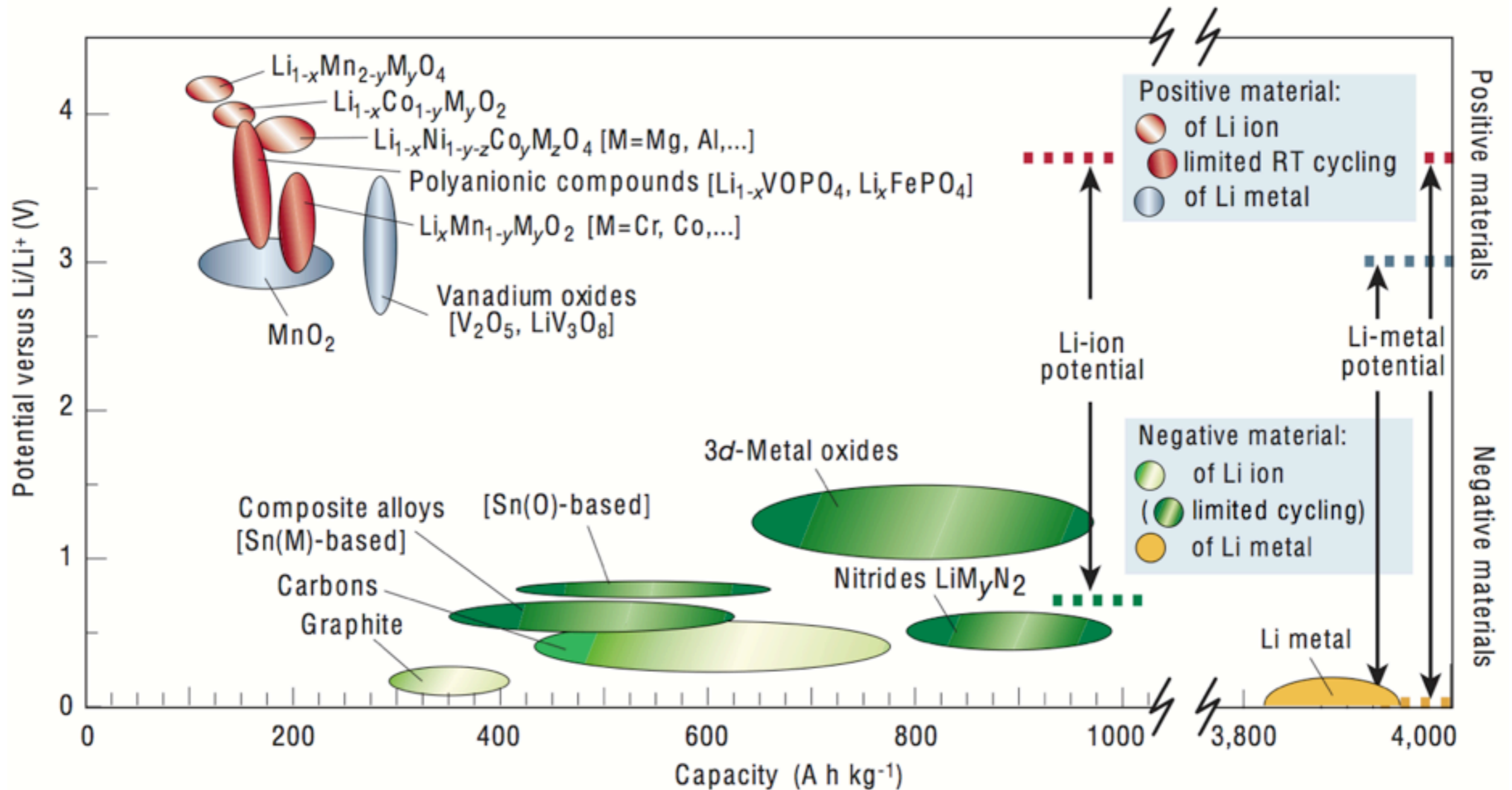
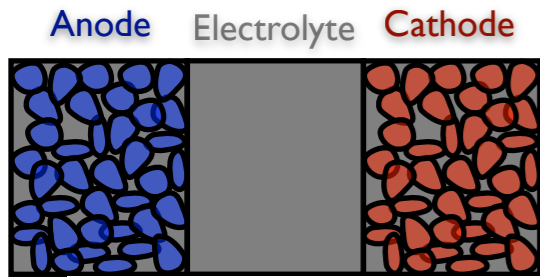
Units:

Wh/kg

# Electrode Materials



# Electrode Materials



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

# Power and Power Density

$$P = \frac{\int_{t_o}^{t_f} I(t)E(t)dt}{(t_f - t_o)M_t}$$

For a composite battery:

$$P = \frac{QE_{ideal}}{W_t(t_f - t_o)} = \min\{Q_c, Q_a\} \frac{E_{ideal}}{W_t(t_f - t_o)}$$

$$= \frac{E_c - E_a}{W_t(t_f - t_o)} zF c_T^i (1 - \epsilon_i - \epsilon_f) h_i$$

# Energy and Energy Density

$$U = \frac{\int_{t_0}^{t_f} I(t)E(t)dt}{M_t}$$

For a composite battery:

$$\begin{aligned} U &= \frac{QE_{ideal}}{M_t} = \min\{Q_c, Q_a\} \frac{E_{ideal}}{W_t} \\ &= \frac{E_c - E_a}{W_t} zF c_T^i (1 - \epsilon_i - \epsilon_f) h_i \end{aligned}$$

# Ragone Plot

