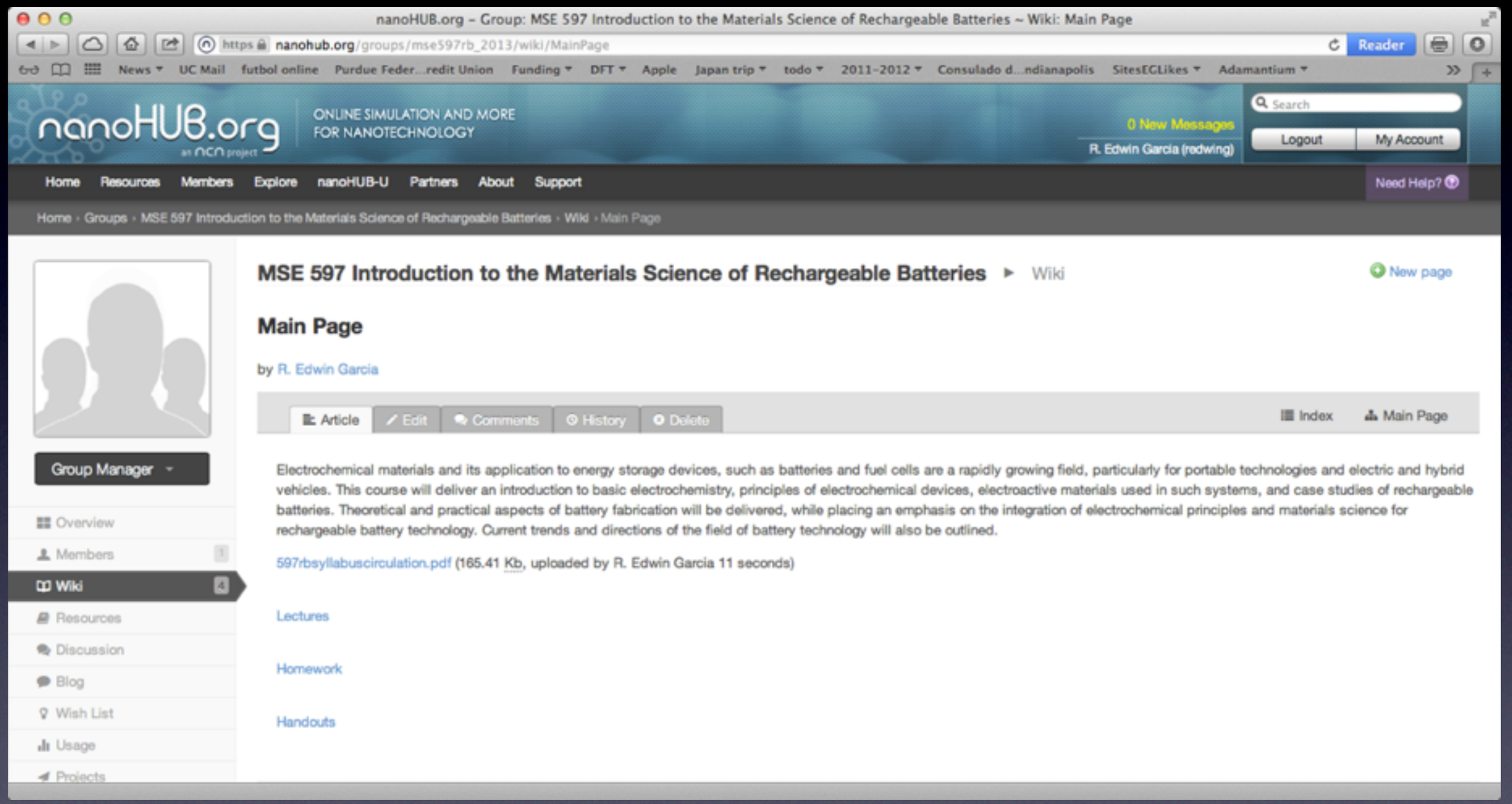
Class Webpage



https://nanohub.org/groups/mse597rb_2013/

Groundwork and Basic Definitions I

Lectures 2 - 4

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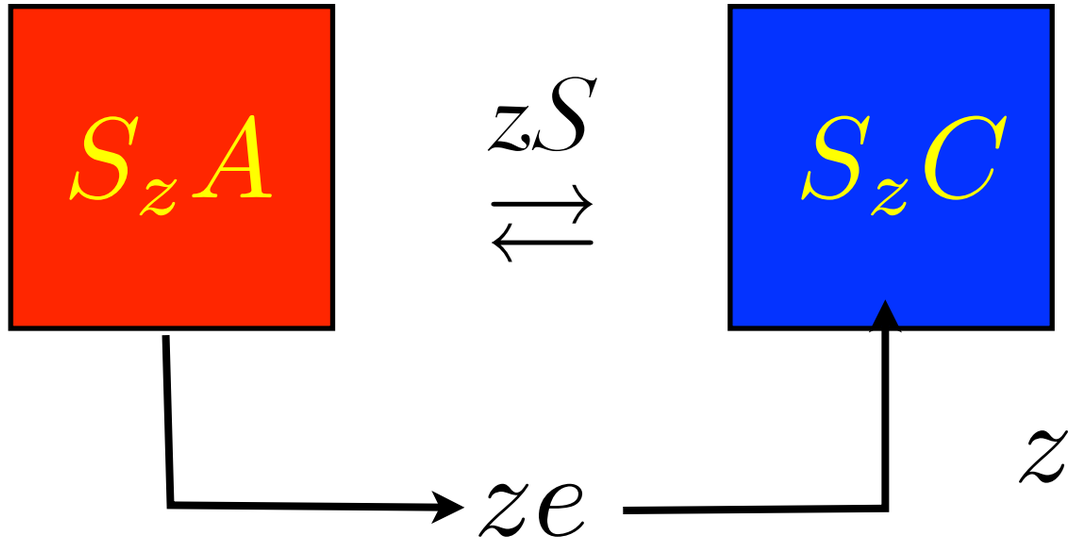
A Sketch of a Rechargeable Battery

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

$$S_zA \rightleftarrows zS + A$$



$$zS + C \rightleftarrows S_zC$$

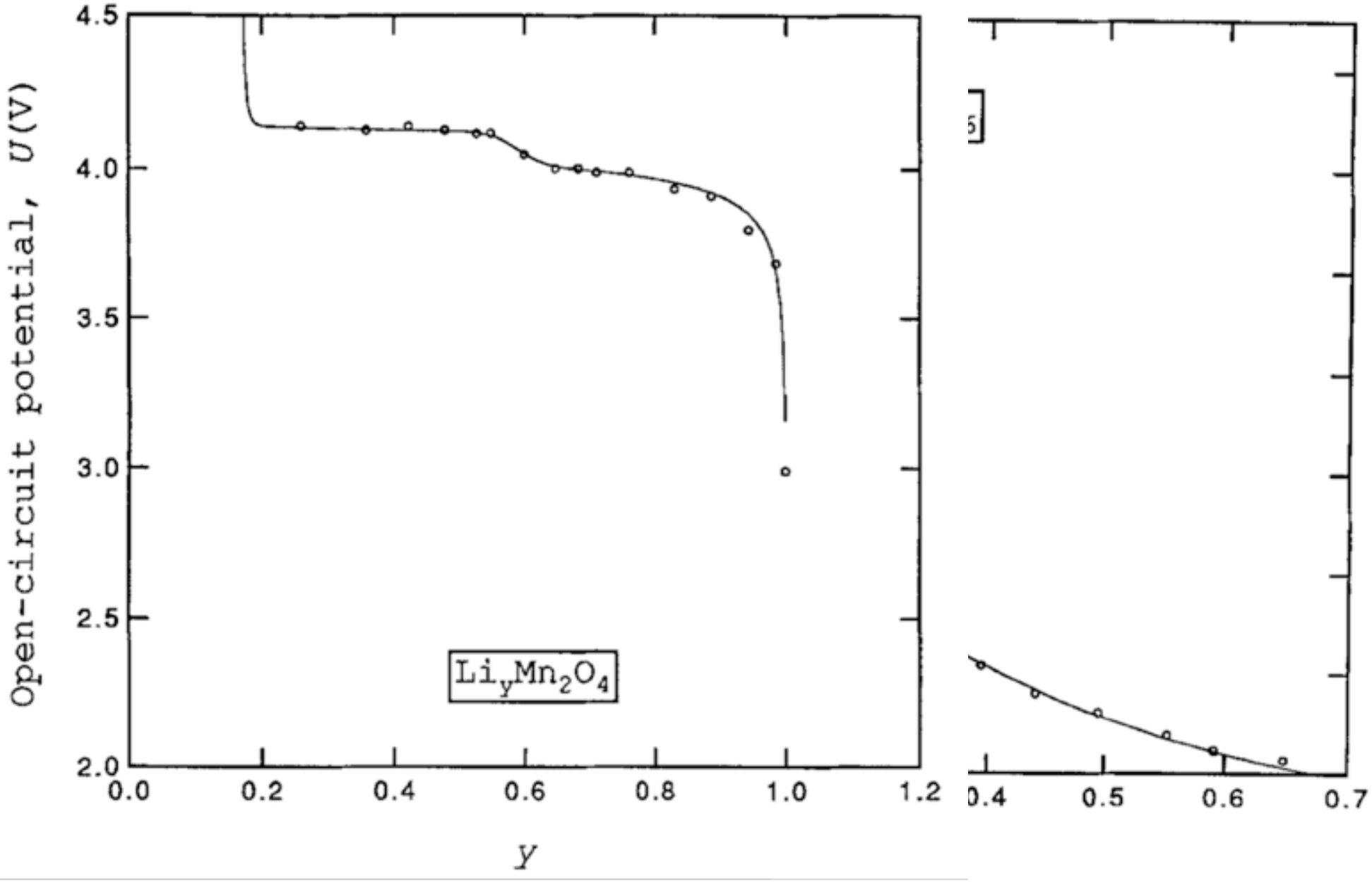
$$zS^+ + C + ze^- \rightleftarrows S_zC$$

Example Reactions

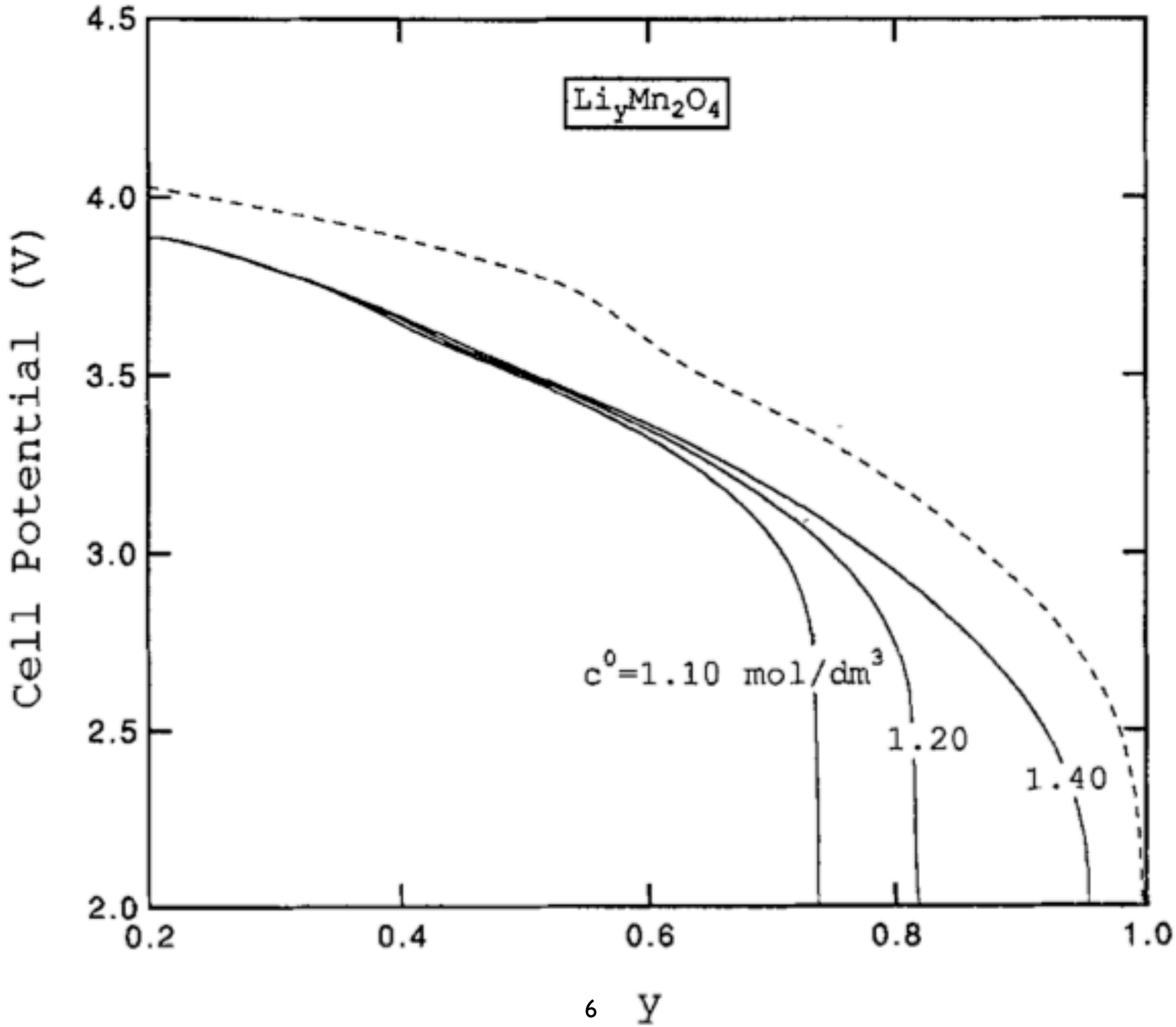
	(–) $Li_xC \longrightarrow C + xLi^+ + xe$	$\varphi^\circ = -2.90$ V	(1)
Li-ion	(+) $Li_{1-x}CoO_2 + xLi^+ + xe \longrightarrow LiCoO_2$	$\varphi^\circ = 1.20$ V	(2)
	(o) $Li_xC + Li_{1-x}CoO_2 \longrightarrow C + LiCoO_2$	$E^\circ = 4.10$ V	(3)

F. Cheng, J. Liang, Z. Tao, and J. Chen "*Functional Materials for Rechargeable Batteries*." Adv. Mater. 2011, 23, 1695–1715.

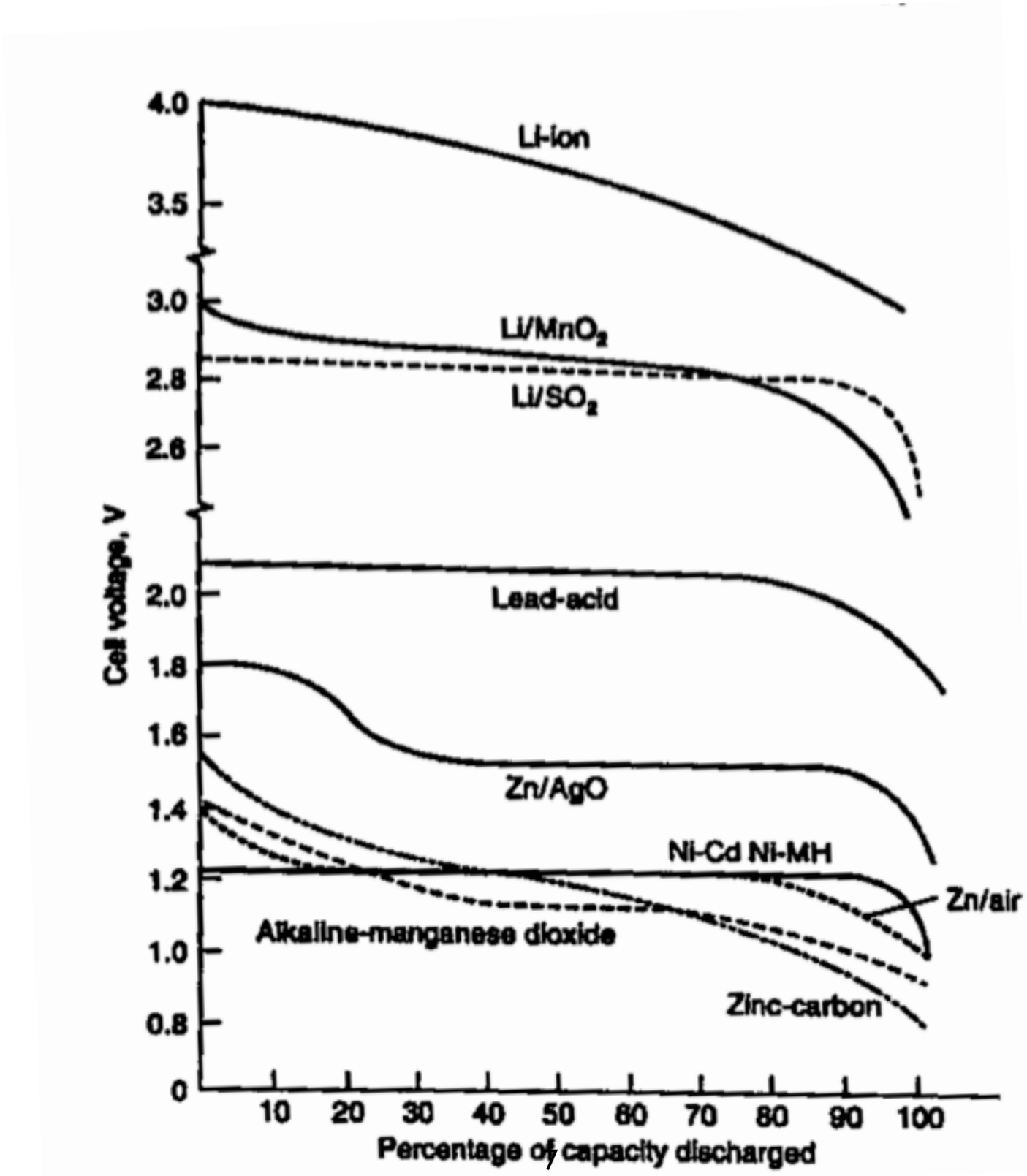
Battery Voltage



Capacity Curve



Battery Voltage



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

Battery Capacity

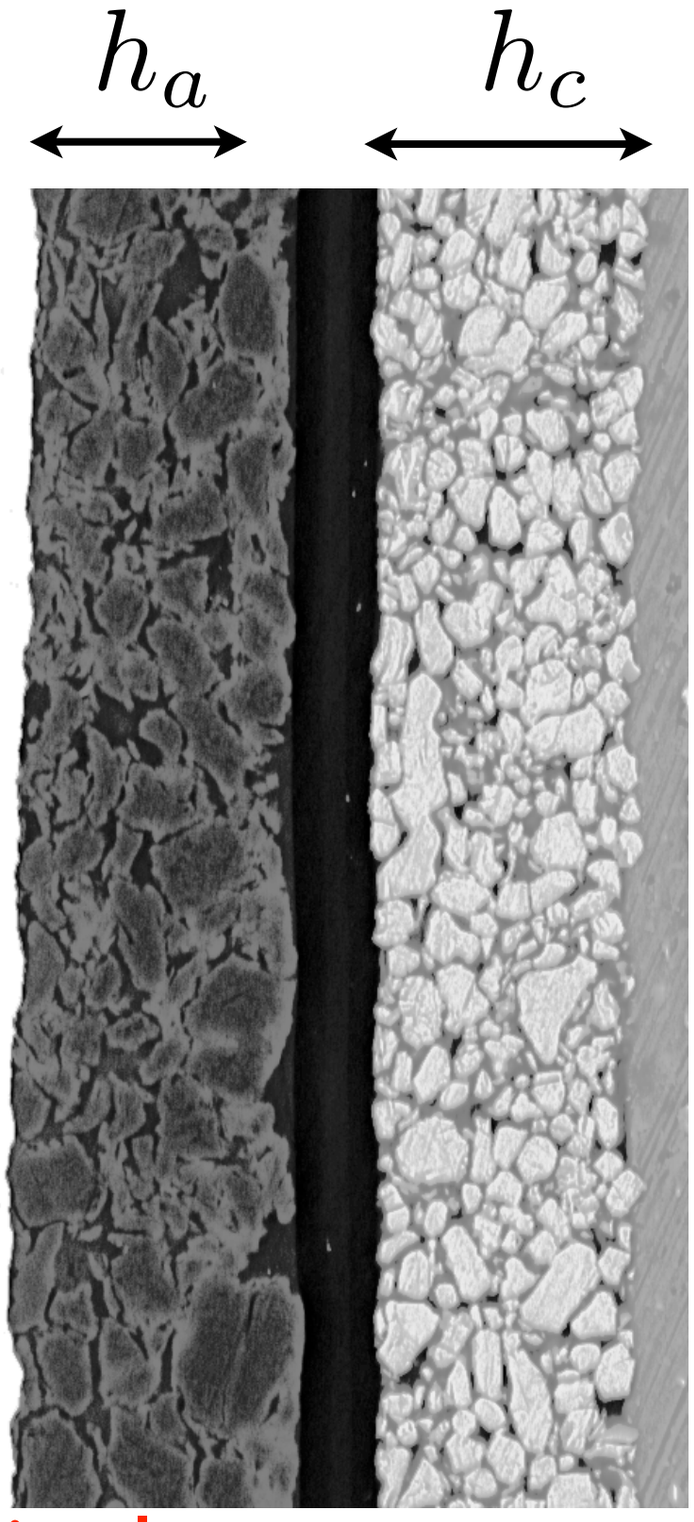
For the Entire Device

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

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

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

Maximum Theoretical Specific Energy

(MTSE)

For an electrode phase

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

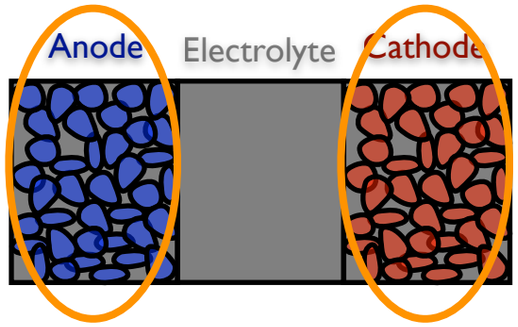
For an entire battery

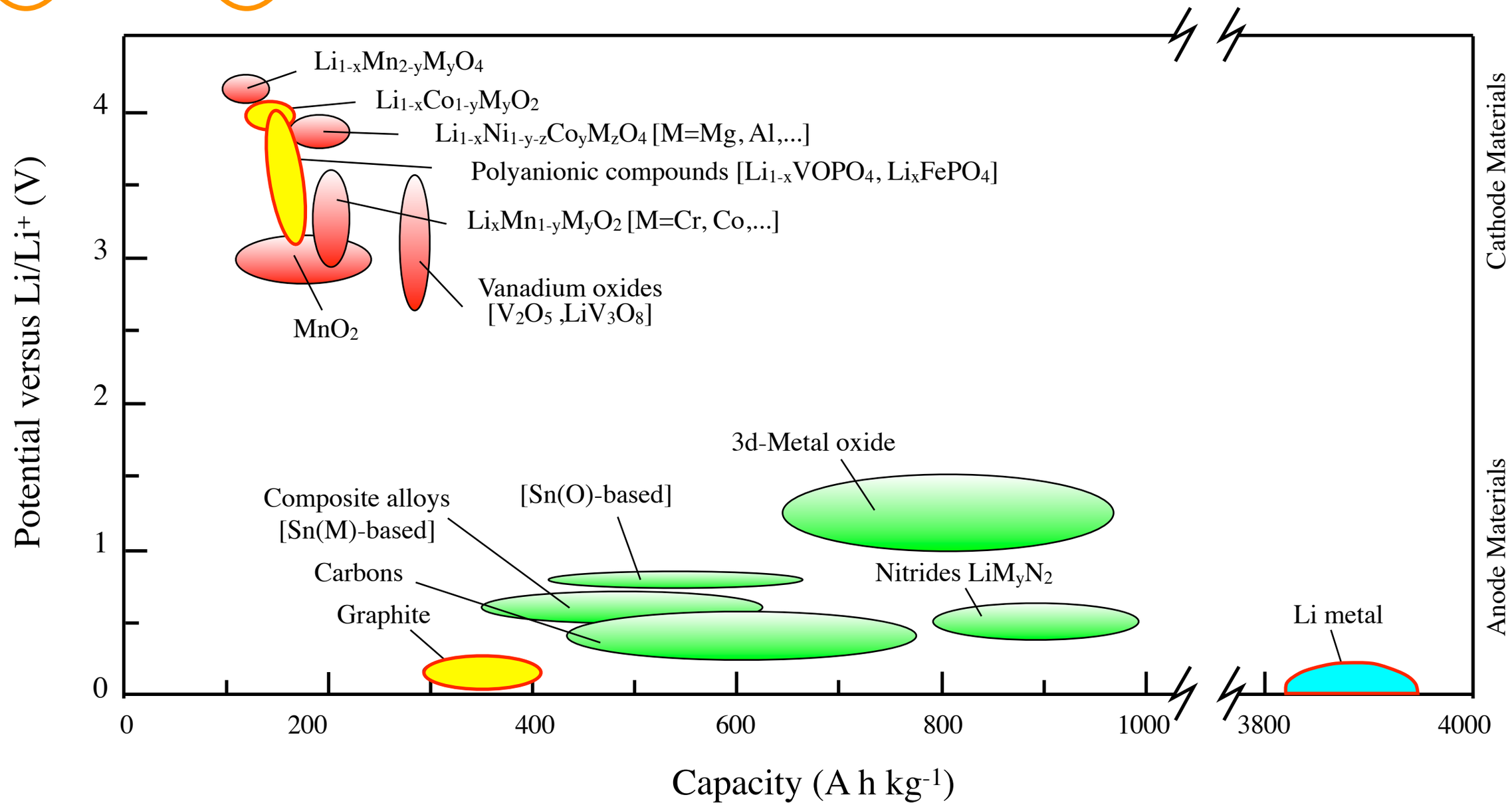
$$MTSE_B = \frac{\min\{Q_c, Q_a\}(Ec - E_a)}{M_{tot}}$$

Units:

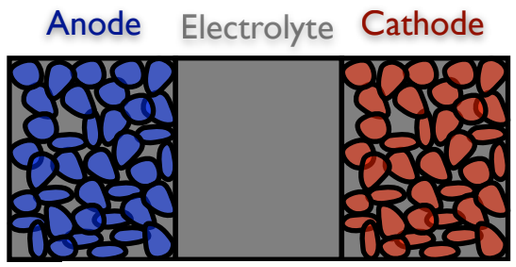
W h/kg

Electrode Materials

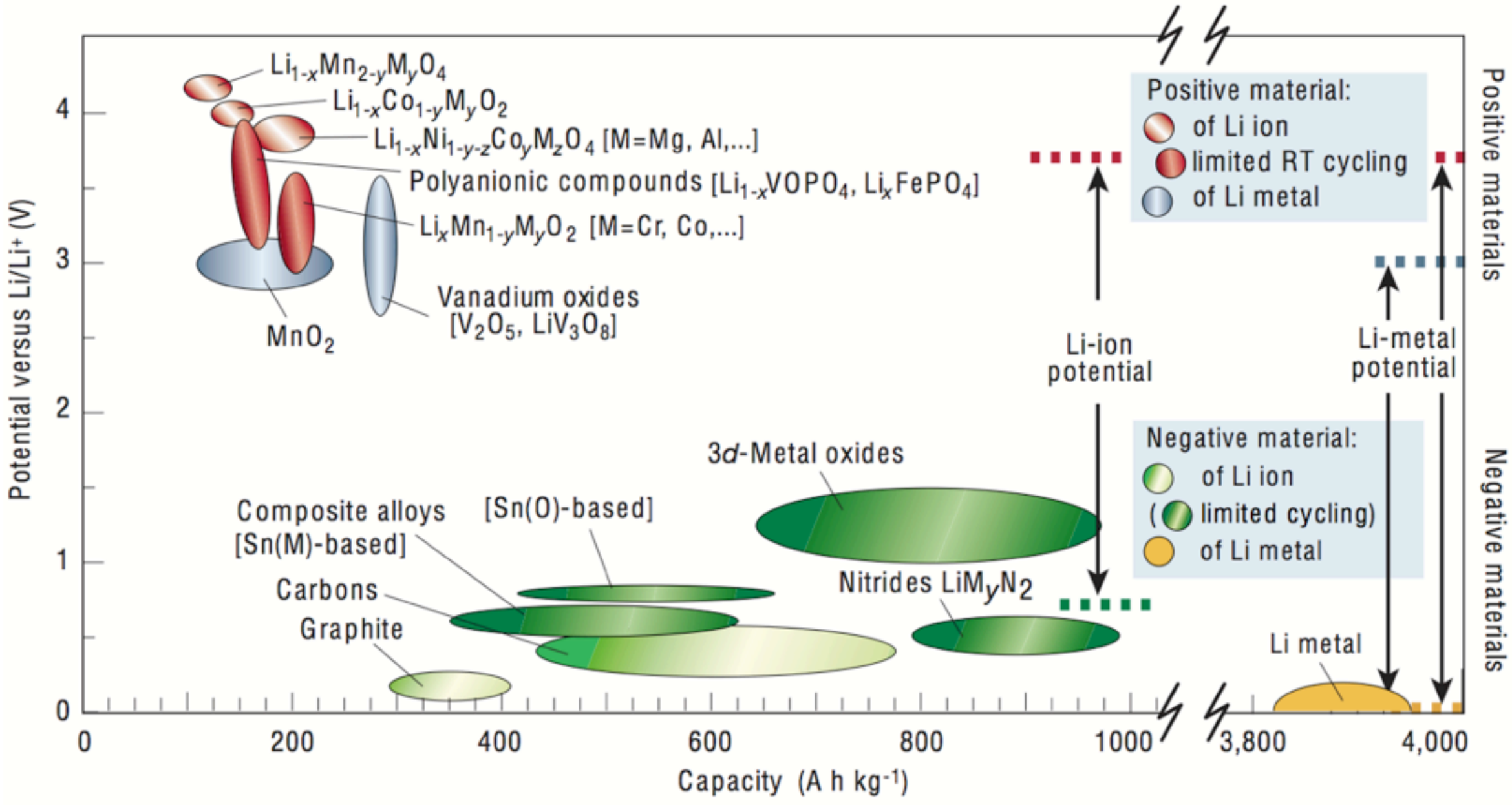




J. M. Tarascon and M. Armand. Issues and Challenges Facing Rechargeable Lithium Batteries. Nature, 414:359-367, 2001



Electrode Materials



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Power and Power Density

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

For a composite battery:

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

$$= \frac{E_c - E_a}{W_t(t_f - t_\circ)} zFc_T^i(1 - \epsilon_i - \epsilon_f)h_i$$

Energy and Energy Density

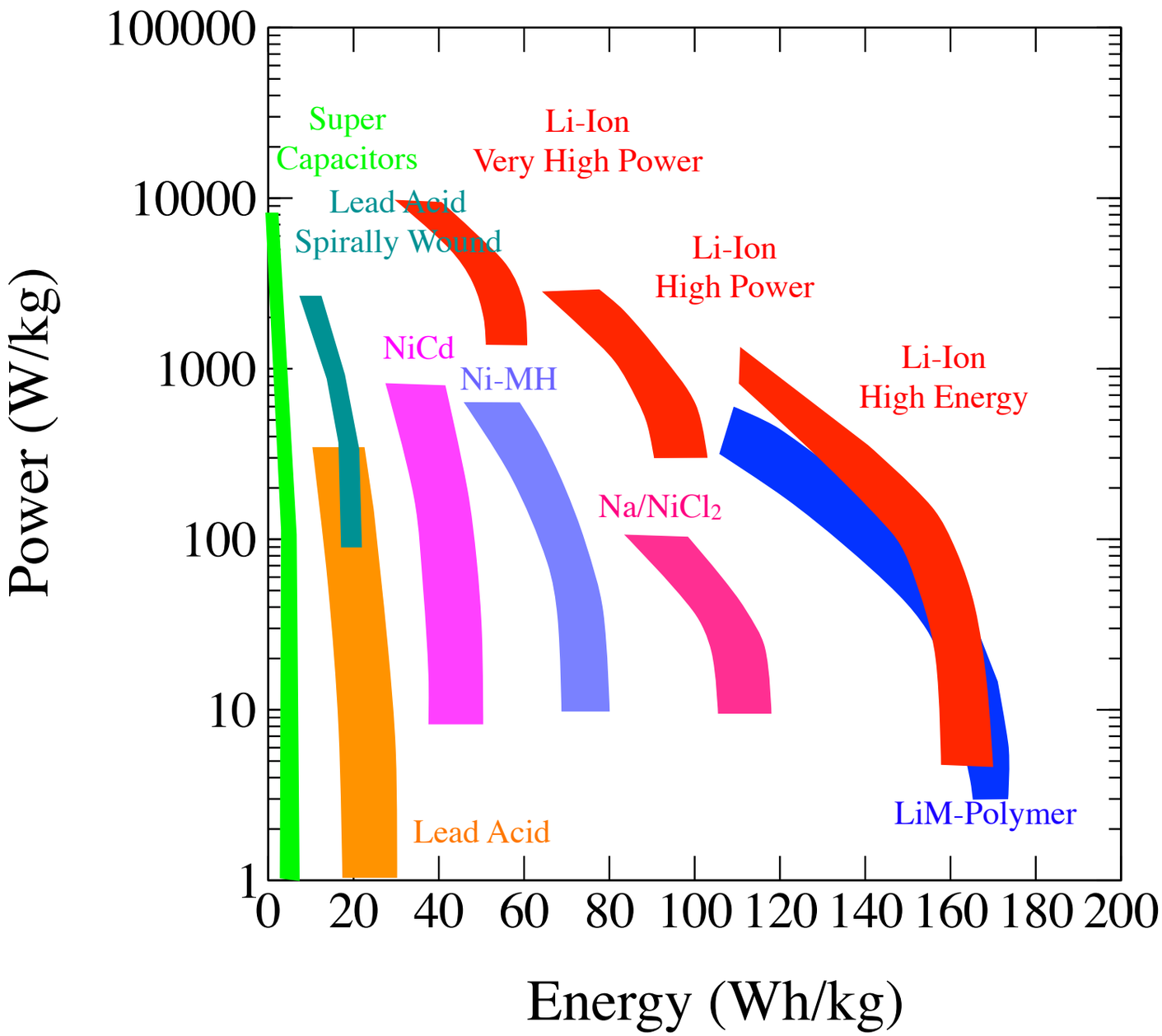
$$U = \frac{\int_{t_\circ}^{t_f} I(t)E(t)dt}{M_t}$$

For a composite battery:

$$U = \frac{QE_{ideal}}{M_t} = \min\{Q_c, Q_a\}\frac{E_{ideal}}{W_t}$$

$$= \frac{E_c - E_a}{W_t} zFc_T^i(1 - \epsilon_i - \epsilon_f)h_i$$

Ragone Plot



R. Brodd. Broddside. In Drug Discovery Approach to Breakthroughs in Batteries, Massachusetts Institute of Technology, Cambridge, Massachusetts, 2008.