Battery Systems Introduction

TSFS19 Battery Systems - Lecture 1

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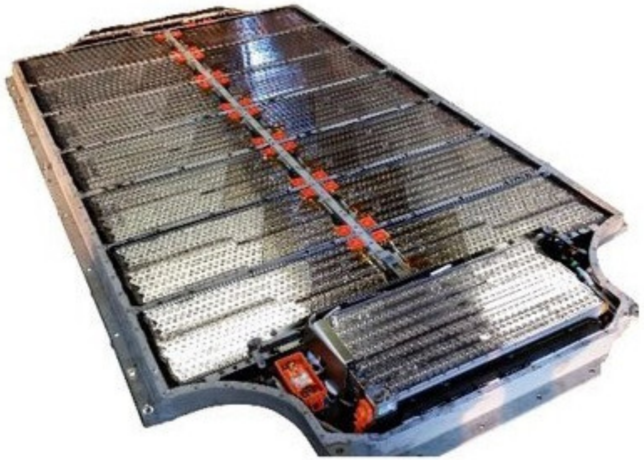
Today's lecture

- Course information
- Introduction of batteries
- Basics of battery chemistry
- Theoretical properties of the cell
    - The electromotive force of the cell (emf)
    - Theoretical charge density and energy density



Course Introduction

Battery Systems, 6 hp

Main field of study: Electrical Engineering Mechanical Engineering

Course level: Second cycle, Advanced

Advancement level: A1

Course type: Programme course

Examiner: Mattias Krysander

Director of studies or equivalent: Johan Löfberg

Education components

- Preliminary scheduled hours: 58 h
- Recommended self-study hours: 102 h
- Total 160 h

Course offered for (8th Semester):

- D — Computer Science and Engineering
- EMM — Energy - Environment - Management
- M — Mechanical Engineering
- Y — Applied Physics and Electrical Engineering
- MEC — Mechanical Engineering

Given first time: 2025 VT2

Prerequisites: Introductory courses in electricity, automatic control, mathematical programming, and probability theory.

Examination

LAB1	4 computer labs	4 hp	U, G
TEN1	A written exam	2 hp	U, 3, 4, 5

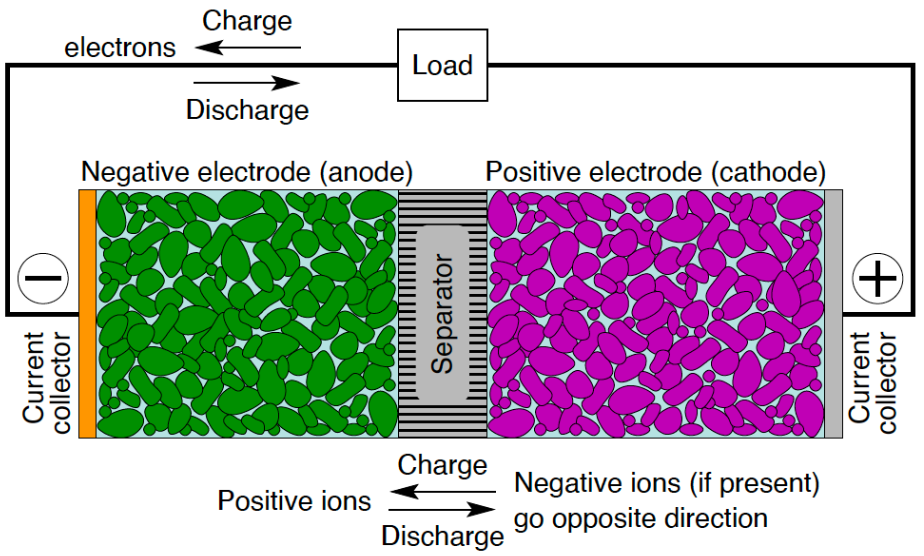
Prerequisites

- Introductory courses in electricity,
- automatic control,
- mathematical programming, and
- probability theory.

Intended Learning Outcomes

An overarching goal is to be able to solve systems engineering problems for battery systems. After completing the course, the student should be able to:

- Describe and perform basic calculations for the construction, function, safety, and reliability of battery systems.
- Mathematically model, parameterize, and simulate batteries.
- Implement and evaluate battery management system functions.

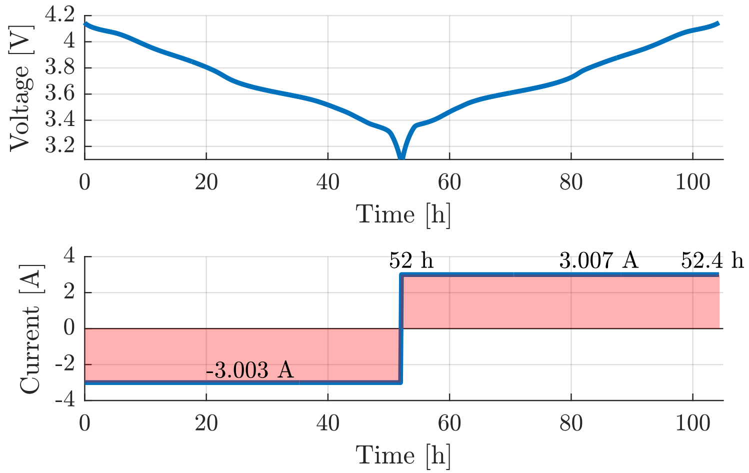


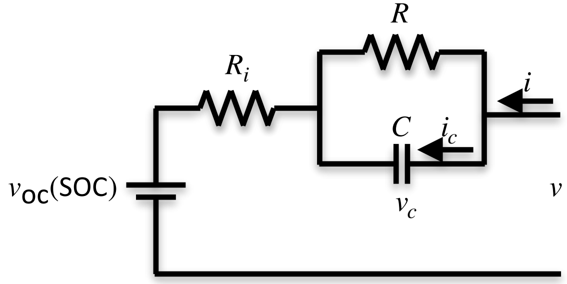
Teaching and Working Methods

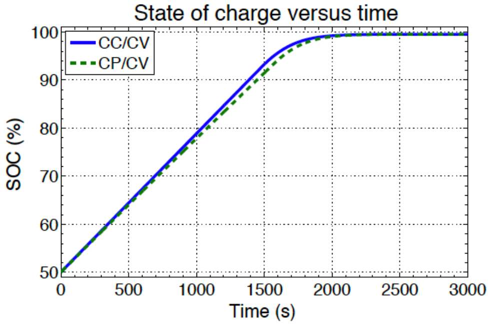
- 10 Lectures
- 9 Exercise sessions (Computers will be needed with Matlab and Python)
- 4 Computer labs (2+2h each)
  - Pairwise, it is possible to prepare at home.
  - Matlab/python
  - Tutoring and examination on the scheduled occasions.
    - Typically, run code, show result plots, numbers, etc. Be ready to explain your solution.
- Written exam (4h)
  - Individual with pen and paper

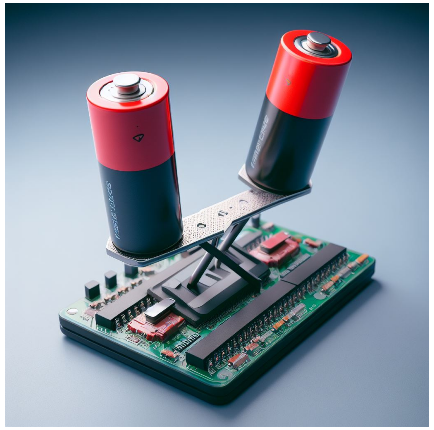
Computer Labs

- **Battery Modeling:** Develop a mathematical model using current and voltage data.
- **SOC Estimation:** Develop estimators for state of charge.
- **Simulation:** Simulate charging, discharging, and battery pack behavior.
- **Electric vehicle application:** Simulate and evaluate battery pack performance.









Course page

TSFS19: Battery Systems

This repository includes lecture notes, material for exercise sessions, computer labs, links to reading material, and other course material. Information here will be added during the course, and you can always get the latest version of course material here.

The course consists of lectures, exercise sessions, computer labs, and a written examination.

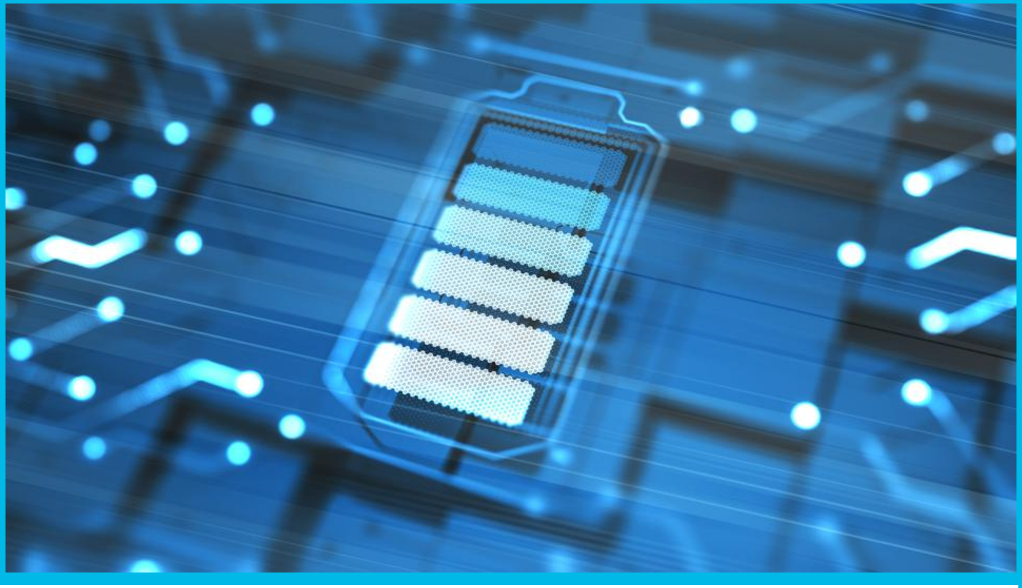
Table of Contents

https://gitlab.liu.se/vehsys/tsfs19

Lecture Plan

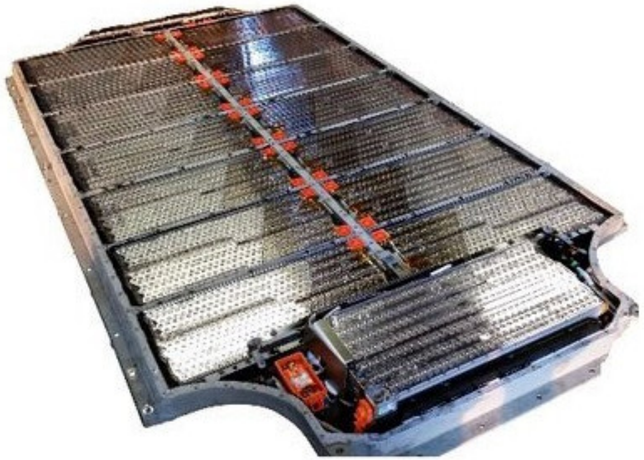
The table below shows the lecture plan for the course. The lecture slides and notes will be added to the Lectures folder during the course. The column "Prep for" indicates which exercise sessions and computer labs you should be prepared for after attending the corresponding lecture. The table also includes recommended reading materials, which are not mandatory but can enhance your understanding of the course content. EE stands for the book "Electrochemical Engineering" by Tomas Fuller and John Harb. Reading material is provided in the Lisam.

Battery - introduction



Introduction

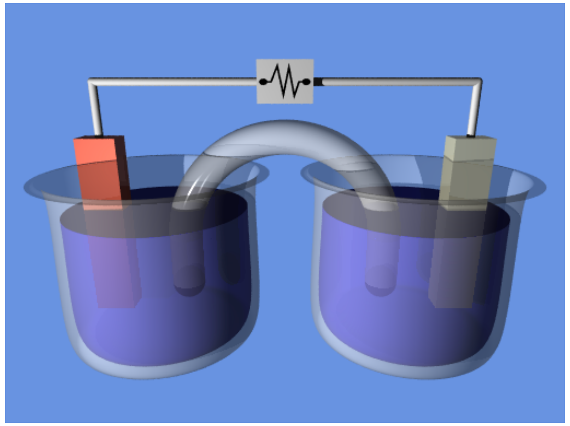
- Batteries are important components in future environmentally friendly energy solutions in transport and energy storage.
- Batteries are an important part of portable electronics.



Batteries

A battery

- converts chemical energy into electrical energy through a reduction-oxidation reaction (redox)
- consists of one or more electrochemical cells.



Cells

- Anode (negative electrode). Electrons are emitted to the external circuit when the electrode is oxidized. (Discharge)
- Cathode (positive electrode). Electrons are absorbed from the external circuit when the electrode is reduced.
- Electrolyte (ion conductor). Medium for transport of charged ions between anode and cathode.

Battery types - primary cells

- Not rechargeable
- Paste-like electrolyte (dry cell)
- Cheap, lightweight
- Used for portable electronics, flashlights etc
- Can be stored for a long time without being discharged
- High energy density
- No or little maintenance
- Low power

Battery types - secondary cells

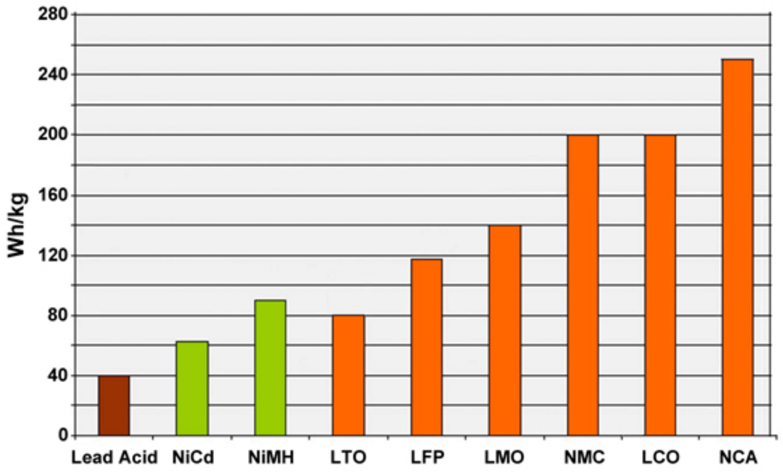
- Rechargeable
- Energy storage (backup for solar cells, vehicles)
- High power density
- High discharge current
- Low energy density
- Higher leakage currents

Basics of battery chemistry

Battery chemistry

Chemical	Anode	Cathode	V	Wh/kg
Primary cells:				
Alkaline MnO_2	Zn	MnO_2	1.5	145
Li/FeS_2	Li	FeS_2(iron sulfide)	1.5	260
Secondary cells:				
Lead Acid	Pb	PbO_2	2	35-40
Nickel-cadmium	Cd	NiOOH	1.2	40-60
Nickel metal hydride	MH	NiOOH	1.2	60-120
Litium-ion (Li-ion)	Li_xC_6	$Li_{(1-x)}CoO_2$	3.6	100-265

MH - hydrogen-absorbent metal mixture

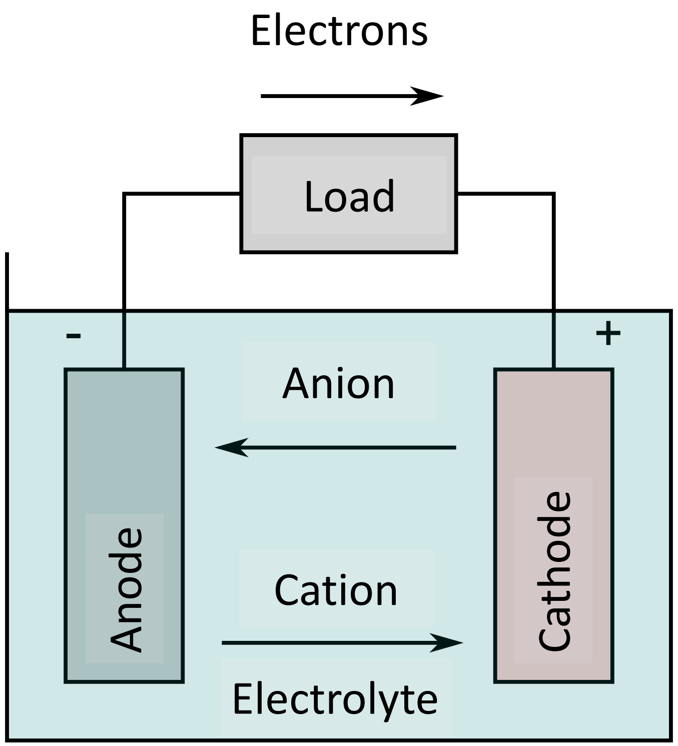


Energy density for different chemistries. Orange bars correspond to various lithium-based chemicals.

Redox reaction in a cell

Electrodes named after the charge sign when discharging.

- Anode
  - negatively charged electrode on discharge
  - the anode material (fuel) is oxidized = emits electrons
- Cathode
  - positively charged electrode on discharge
  - the cathode material absorbs electrons = reduced
- Electrolyte
  - Liquid solution
  - It does not conduct electrons but contains free moving
    - Anion - negatively charged ion
    - Cation - positively charged ion



Redox reaction in a cell

- Anode reaction (negative electrode)

$$bB - ne^- \rightleftharpoons dD$$

  b molecules of B emit n electrons to form d molecules of D

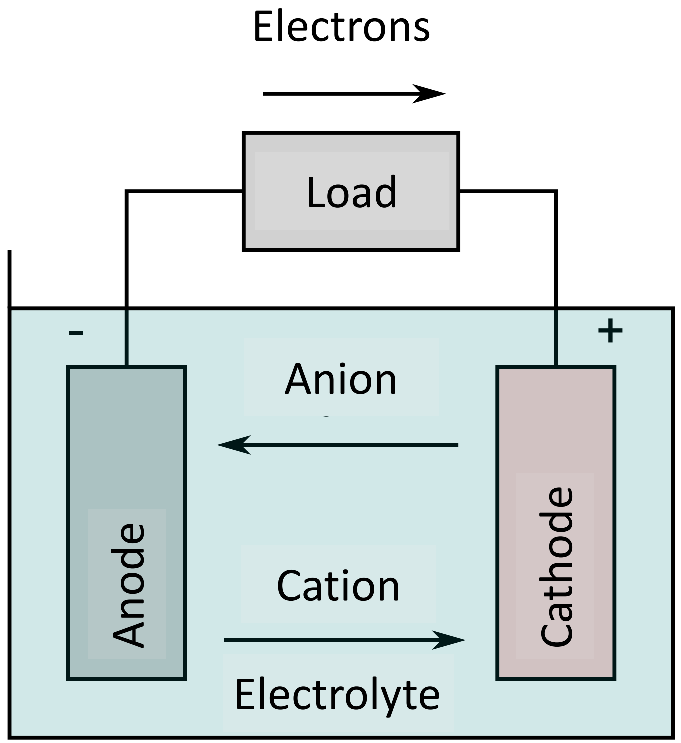
- Cathode reaction (positive electrode)

$$aA + ne^- \rightleftharpoons cC$$

  a molecules of A absorb n electrons to form c molecules of C

- Cell reaction

$$aA + bB \rightleftharpoons cC + dD$$



Reduction of the Gibbs free energy is the driving force of the reaction.

- function of concentration of reactants, products, and temperature
- gives the cell's electromotive force (emf) = voltage

Reactions are balanced on
- atomic species
- charge

NiCd-cell - Discharge

- Power is emitted in the load
- Anode reaction: Cadmium (metal) is oxidized to form cadmium hydroxide

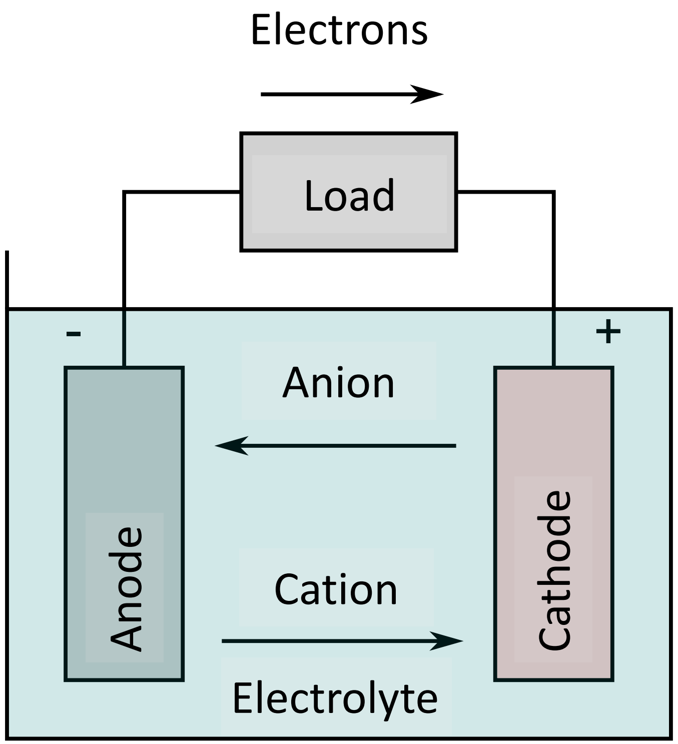
$$Cd + 2OH^{-} \rightarrow Cd(OH)_2 + 2e^{-}$$

- Cathode reaction: Nickel oxide hydroxide is reduced to nickel hydroxide

$$NiO(OH)(s) + H_2 0 + e^{-} \rightarrow OH^{-} + Ni(OH)_2(s)$$

- Full cell reaction:

$$Cd + 2NiO(OH)(s) + 2H_2 0 \rightarrow Cd(OH)_2 + 2Ni(OH)_2(s)$$



NiCd-cell - Charging

- DC power source drives current in the opposite direction
- Anode reaction: Cadmium hydroxide is reduced to cadmium metal

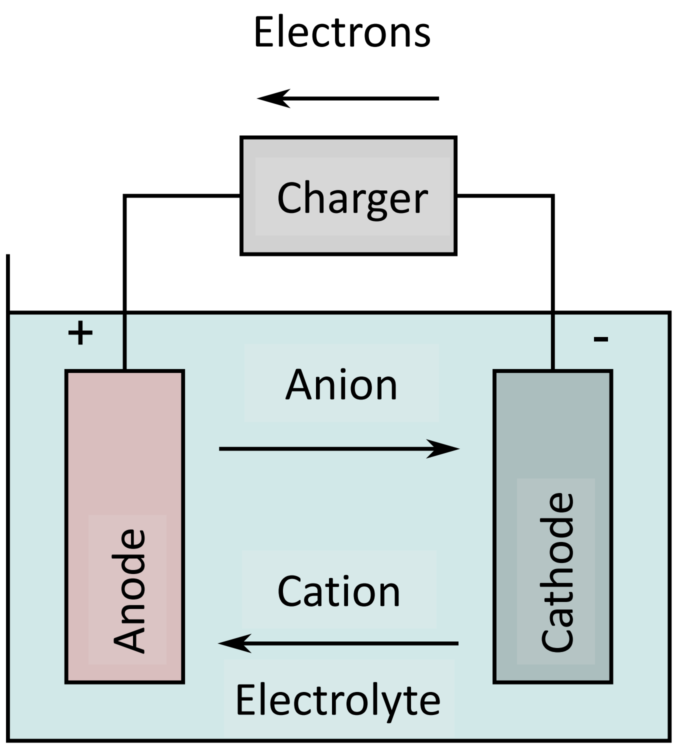
$$Cd + 2OH^- \leftarrow Cd(OH)_2 + 2e^-$$

- Cathode reaction: Nickel hydroxide is oxidized to nickel oxyhydroxide

$$NiO(OH)(s) + H_20 + e^- \leftarrow OH^- + Ni(OH)_2(s)$$

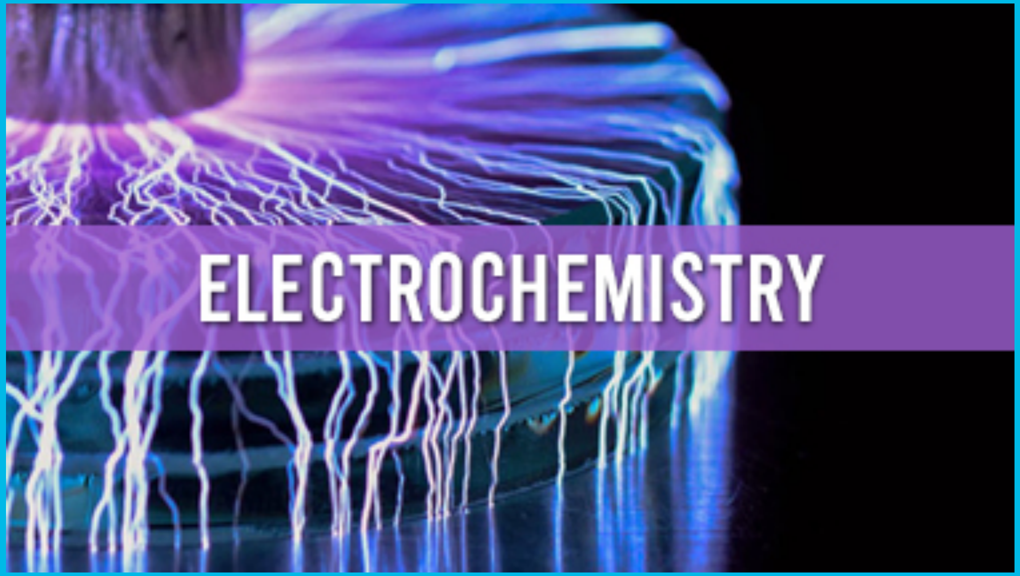
- Cellreaktionen

$$Cd + 2NiO(OH)(s) + 2H_20 \leftarrow Cd(OH)_2 + 2Ni(OH)_2(s)$$



Theoretical properties of the cell

Voltage, charge density and energy content



Properties of Electrochemical Systems

- *Current* I, Ampere [A]
- *Charge* Q, Coulomb [C = As]. Commonly expressed in Ah
- $Q = \int i(t)dt$, for constant current I => $Q = It$
- *The elementary charge* is the electric charge of one electron: $q_e = 1.602 \cdot 10^{-19}$ C
- The *Avogadros constant* is the number of particles per mole $N_A = 6.022 \cdot 10^{23}$ mol^{-1}
- *Faraday constant* defines the charge of 1 mole of electrons:

$$F = q_e N_A = 96485 \text{ C/mol} = \frac{96485 \text{ As/mol}}{3600 \text{ s/h}} = 26.8 \text{ Ah/mol}$$

Cell Potential (Open circuit voltage)

Standard potential for half cells

- Potential in relation to hydrogen = normal potential
- Plus pole: half cell with the highest normal potential

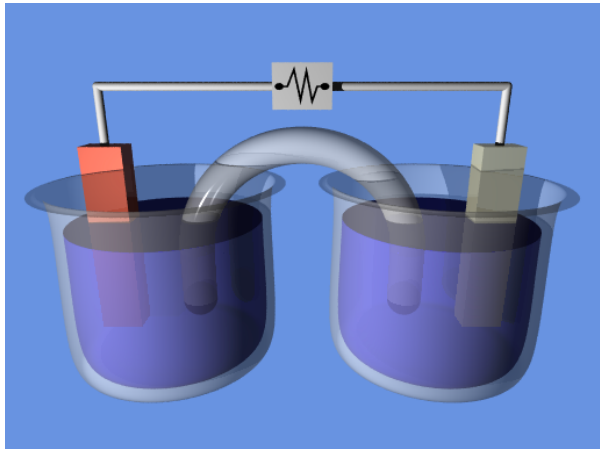


TABLE 17.1 Standard Reduction Potentials at 25 °C

	Reduction Half-Reaction		U^0(v)	
Stronger oxidizing agent	$F_2(g) + 2e^-$	$\longrightarrow 2F^-(aq)$	2.87	Weaker reducing agent
	$H_2O_2(aq) + 2H^+(aq) + 2e^-$	$\longrightarrow 2H_2O(l)$	1.78	
	$MnO_4^-(aq) + 8H^+(aq) + 5e^-$	$\longrightarrow Mn^{2+}(aq) + 4H_2O(l)$	1.51	
	$Cl_2(g) + 2e^-$	$\longrightarrow 2Cl^-(aq)$	1.36	
	$Cr_2O_7^{2-}(aq) + 14H^+(aq) + 6e^-$	$\longrightarrow 2Cr^{3+}(aq) + 7H_2O(l)$	1.33	
	$O_2(g) + 4H^+(aq) + 4e^-$	$\longrightarrow 2H_2O(l)$	1.23	
	$Br_2(aq) + 2e^-$	$\longrightarrow 2Br^-(aq)$	1.09	
	$Ag^+(aq) + e^-$	$\longrightarrow Ag(s)$	0.80	
	$Fe^{3+}(aq) + e^-$	$\longrightarrow Fe^{2+}(aq)$	0.77	
	$O_2(g) + 2H^+(aq) + 2e^-$	$\longrightarrow H_2O_2(aq)$	0.70	
	$I_2(s) + 2e^-$	$\longrightarrow 2I^-(aq)$	0.54	
	$O_2(g) + 2H_2O(l) + 4e^-$	$\longrightarrow 4OH^-(aq)$	0.40	
	$Cu^{2+}(aq) + 2e^-$	$\longrightarrow Cu(s)$	0.34	
	$Sn^{4+}(aq) + 2e^-$	$\longrightarrow Sn^{2+}(aq)$	0.15	
	$2H^+(aq) + 2e^-$	$\longrightarrow H_2(g)$	0	
	$Pb^{2+}(aq) + 2e^-$	$\longrightarrow Pb(s)$	- 0.13	
	$Ni^{2+}(aq) + 2e^-$	$\longrightarrow Ni(s)$	- 0.26	
	$Cd^{2+}(aq) + 2e^-$	$\longrightarrow Cd(s)$	- 0.40	
	$Fe^{2+}(aq) + 2e^-$	$\longrightarrow Fe(s)$	- 0.45	
	$Zn^{2+}(aq) + 2e^-$	$\longrightarrow Zn(s)$	- 0.76	
	$2H_2O(l) + 2e^-$	$\longrightarrow H_2(g) + 2OH^-(aq)$	- 0.83	
	$Al^{3+}(aq) + 3e^-$	$\longrightarrow Al(s)$	- 1.66	
	$Mg^{2+}(aq) + 2e^-$	$\longrightarrow Mg(s)$	- 2.37	
	$Na^+(aq) + e^-$	$\longrightarrow Na(s)$	- 2.71	
Weaker oxidizing agent	$Li^+(aq) + e^-$	$\longrightarrow Li(s)$	- 3.04	Stronger reducing agent

Table 17-1 Chemistry, 5/e

The reaction with the lowest standard potential becomes the negative pole and proceeds reverse during discharge.

Calculate the emf of a ZnCu cell

- Cell reaction

$$Cu^{2+}(aq) + Zn(s) \rightarrow Cu(s) + Zn^{2+}(aq)$$

- Anode reaction / negative pole

$$Zn(s) \rightarrow Zn^{2+}(aq) + 2e^{-} \;\Rightarrow\; U_{-}^{0} =$$

- Cathode reaction / positive pole

$$Cu^{2+}(aq) + 2e^{-} \rightarrow Cu(s) \;\Rightarrow\; U_{+}^{0} =$$

The largest standard potential becomes the positive pole

- Emf for the ZuCu cell

$$U_{\text{cell}}^{0} = U_{+}^{0} - U_{-}^{0} =$$

Calculate the emf of a ZnCu cell

- Cell reaction

$$Cu^{2+}(aq) + Zn(s) \rightarrow Cu(s) + Zn^{2+}(aq)$$

- Anode reaction / negative pole

$$Zn(s) \rightarrow Zn^{2+}(aq) + 2e^{-} \;\Rightarrow\; U_{-}^{0} = -\,0.76\text{V}$$

- Cathode reaction / positive pole

$$Cu^{2+}(aq) + 2e^{-} \rightarrow Cu(s) \;\Rightarrow\; U_{+}^{0} = 0.34\text{V}$$

The largest standard potential becomes the positive pole

- Emf for the ZuCu cell

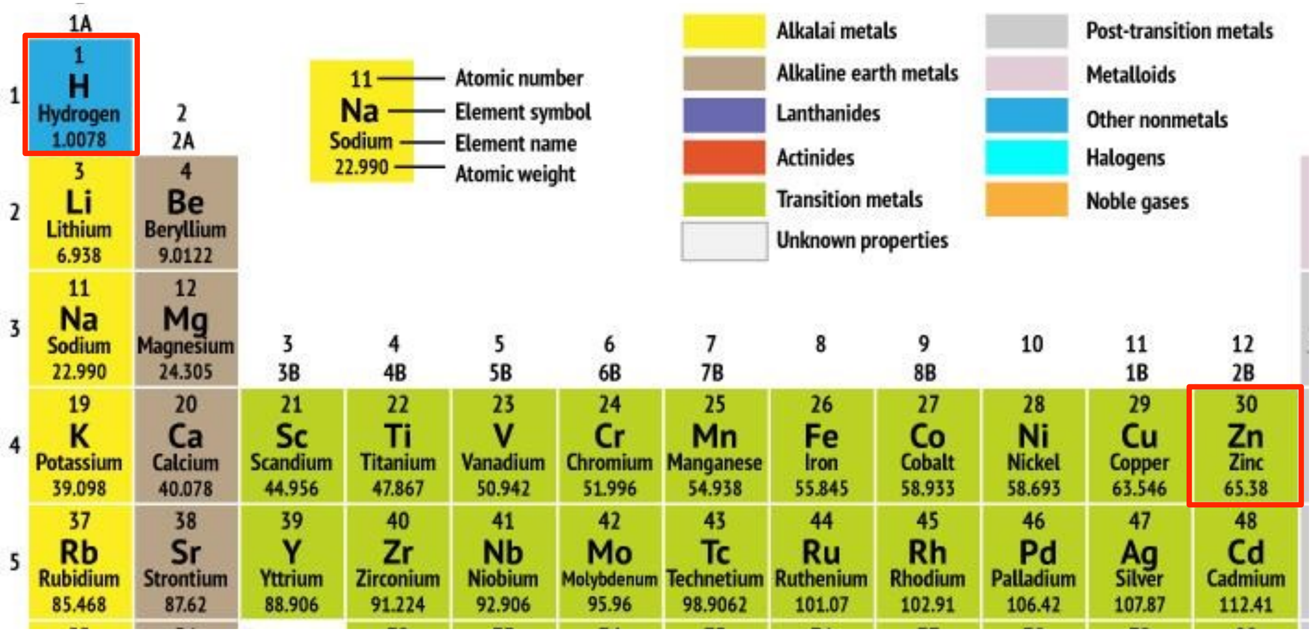
$$U_{\text{cell}}^{0} = U_{+}^{0} - U_{-}^{0} = 0.34 - (-0.76) = 1.1\text{V}$$

Charge and Energy Density

Properties of Electrochemical Systems

- The *molar mass* M_i of a compound i is equal to the sum of the *atomic masses* of its constituent atoms in g/mol.
- Ex: The molar mass of zinc is $M_{Zn} = 65.38$ g/mol
- Ex: The molar mass of hydrogen gas H_2 is

$$M_{H_2} = 2M_H = 2.015 \text{ g/mol}$$



Example

Question. How much Zn in the oxidation $Zn(s) \rightarrow Zn^{2+}(aq) + 2e^-$ has reacted in 2 hours if the current is 12 A. Answer in moles and mass of zinc.

Solution. The amount of charge passed is

$$Q = I \cdot t = 12\ \mathrm{C/s} \cdot 2\ \mathrm{h} \cdot 3600\ \mathrm{s/h} = 86{,}400\ \mathrm{C}$$

Each Zn atom corresponds to 2 electrons. Thus, the reacted amount of zinc is

$$n_{Zn} = \frac{Q}{s_{Zn}F} = \frac{86{,}400\ \mathrm{C}}{2\ \mathrm{mol\ e/mol\ Zn} \cdot 96{,}485\ \mathrm{C/mol\ e}} = 0.448\ \mathrm{mol\ Zn}$$

The consumed mass of zinc is the moles times the molecular mass:

$$m_{Zn} = M_{Zn} \cdot n_{Zn} = 65.38\ \mathrm{g/mol\ Zn} \cdot 0.448\ \mathrm{mol\ Zn} = 29.3\ \mathrm{g\ Zn}$$

Faraday Law of Electrolysis

Motivated by the previous example Faraday law can be formulated as

$$m_i = \frac{M_i Q}{nF}, \quad \text{where}$$

- m_i is the mass of species i [g]
- M_i is the molar mass of species i [g/mol]
- Q the passed amount of charge [C]
- n the number of electrons per species i
- F the Faraday constant [C/mol]

Theoretical charge density

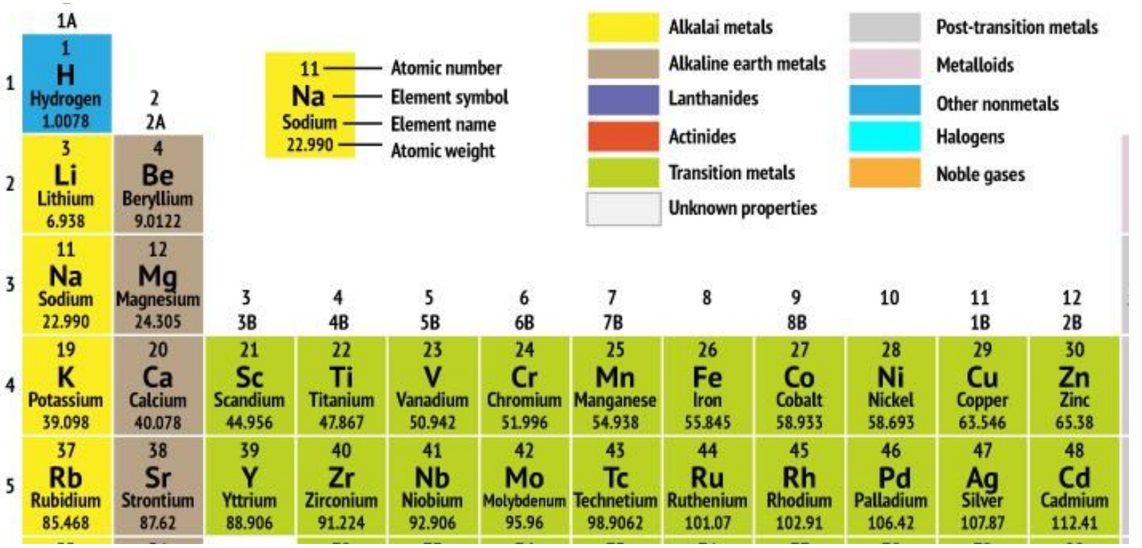
- A measure of the electrochemical capacity of a material is the charge per mass [Ah/g], i.e. its *charge density*.
- Calculation of the charge density of substance A:

$$\frac{Q}{m_A} = \frac{F \cdot n}{M_A} = [\frac{\text{Ah/(mol e)} \cdot \text{(mol e)/(mol A)}}{\text{g/(mol A)}} = \text{Ah/g}]$$

- Example: What is the charge density of Zn?

$$\frac{26.8 \cdot 2\ \text{Ah/mol}}{65.4\ \text{g/mol}} = 0.82\ \text{Ah/g}$$

- How do we include both electrodes?



Theoretical charge density and energy density

- Simply add the mass for both electrodes.
- Use the right amount of material for both the anode and cathode.

$$\left.\frac{g}{Ah}\right|_{cell} = \left.\frac{g}{Ah}\right|_{cathode} + \left.\frac{g}{Ah}\right|_{anode}$$

- Theoretical charge density (specific charge) for a cell

$$\left.\frac{Ah}{g}\right|_{cell} = \left(\left.\frac{g}{Ah}\right|_{cathode} + \left.\frac{g}{Ah}\right|_{anode}\right)^{-1}$$

- The mass of electrolyte, container, contacts is not included.
- Theoretical energy density [Wh / g] is obtained by multiplying that charge density by the emf ([Ah / g · V = Wh / g])

Theoretical energy density - example ZnCu cell

- Cell reaction:

$$Cu^{2+}(aq) + Zn(s) \rightarrow Cu(s) + Zn^{2+}(aq)$$

- Charge density:

$$\frac{Ah}{g} = \left(\overbrace{\frac{63.5\text{g}}{2 \cdot 26.8\text{Ah}}}^{Cu} + \overbrace{\frac{65.4\text{g}}{2 \cdot 26.8\text{Ah}}}^{Zn} \right)^{-1} = 0.42\ \text{Ah/g}$$

- Theoretical energy density:

$$\frac{Wh}{g} = U^0 \frac{Ah}{g} = 1.1\ \text{V} \cdot 0.42\ \text{Ah/g} = 0.46\ \text{Wh/g} = 460\ \text{Wh/kg}$$

Learning Outcomes

- Formulate balanced cell reactions given half-cell reactions.
  - Balance atom species and charge.
- Compute the standard potential of a cell given half-cell potentials: $U^0_{\text{cell}} = U^0_+ - U^0_-$
  - The lowest potential will be the negative electrode and its reaction will be reversed during discharge.
- Understand current: $I = dQ/dt$ [A = C/s]
- Use Faraday's law of electrolysis: $m_i = \dfrac{M_i Q}{nF}$
- Compute charge density for half-cells and cells:

$$\left.\frac{Ah}{g}\right|_A = \frac{F \cdot n}{M_A} \qquad \left.\frac{Ah}{g}\right|_{cell} = \left(\left.\frac{g}{Ah}\right|_{cathode} + \left.\frac{g}{Ah}\right|_{anode}\right)^{-1}$$

- Compute theoretical energy density of a cell = $U^0_{cell} \cdot \left.\dfrac{Ah}{g}\right|_{cell}$ [VAh/g = Wh/g] www.liu.se

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