Sustainable Hydrogen and Electrical Energy Storage, SET3031
Exam 24 June 2009

Question 1.

a. Name potential drawbacks of the large scale use of hydrogen.
b. Future renewable energy sources often produce electricity. Estimate roughly the efficiency of storage and subsequent use of the electrical energy by using hydrogen and by using batteries.
c. Why would a future energy economy use hydrogen as an energy carrier? (name 5 reasons)

Question 2.

a. Indicate five main goals for hydrogen storage in materials. Indicate materials that fulfill these individual goals. Are materials available that fulfill all goals at the same time?
b. Indicate methods of hydrogen storage as a function of increasing interaction strength of hydrogen and the material.

Question 3.

Magnesium can react with hydrogen to form MgH_2. The enthalpy of formation is -77kJ/mol and the weight percentage of H in MgH_2 is 7.6 wt.%.

a. Under which conditions (approximately) is it possible to react Mg and H_2 and thus store hydrogen in MgH_2? Why is this the case?
b. How can you improve the storage characteristics of Mg?
c. What will happen with the temperature of the Mg if you react it with hydrogen and what does that mean for the maximum loading rate?

Question 4.

Consider the standard reduction potentials:

$Fe^{2+} + 2e^- \rightarrow Fe(s)$	-0.44 V
$Cu^{2+} + 2e^- \rightarrow Cu(s)$	+0.337
$Ag^+ + e^- \rightarrow Ag(s)$	+0.799

Assume $Cu^{2+}(aq)$ is dissolved in the electrolyte around an Ag(s) electrode and cannot reach the Fe(s) counter electrode.

a. Write down the total reaction in a battery configuration, and in which direction the reaction will proceed spontaneously.
b. What is the open cell potential under standard conditions, and how much chemical energy is converted to electrical energy per mole reacted Fe(s) ($\Delta G=-(\phi_C-\phi_A)zF$, F=96500 C/mol)?

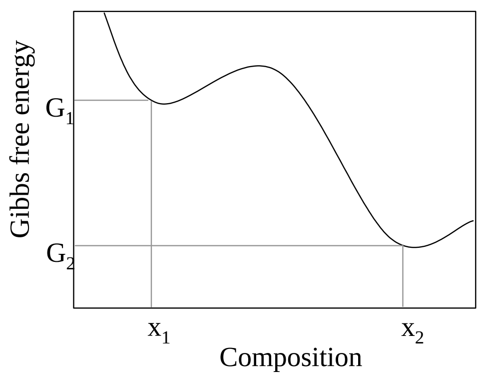
Assume the starting concentrations are $c_{Ag+}=0$, $c_{Fe2+}=0.05$, $c_{Cu2+}=2$ mol/liter and assuming $c_{Cu(s)}=c_{Fe(s)}=c_{Ag(s)}=1$. Nernst law: (Nernst: $\varepsilon = (\phi_C - \phi_A) = \varepsilon^o - (RT/zF)\,[\ln \Pi c_j^{\nu}]$, for example applied to the half reaction $Fe^{2+}(aq) + 2e^- \rightarrow Fe(s)$ leads to $\varepsilon = \varepsilon^o - (RT/2F)\ln(c_{Fe(s)}/c_{Fe2+})$ where R=8.31 J/(mol K), T=293 K.

c. Calculate the open cell potential between the two electrodes under the given conditions.
d. When does the reaction stop?

e. Describe qualitatively what would happen if there is initially an amount of Ag^{+}(aq) in the electrolyte.

Question 5.

a. Give five required properties for rechargeable batteries.
b. Explain how a Li-ion battery works, what are the components, and what is their function?
c. Which part of a Li-ion battery generally restricts the power-density in the case of host reactions?
d. Discuss two different origins of reduced cycle life in Li-ion electrode host reactions.
e. Give the definition of the chemical potential in relation to the Gibbs free energy, and the role in a battery.
f. Sketch chemical potential as a function of composition for the Gibbs energy shown in the graph, and explain its behavior.
g. What can you say about the voltage during (dis)charge between the compositions x_1 and x_2?



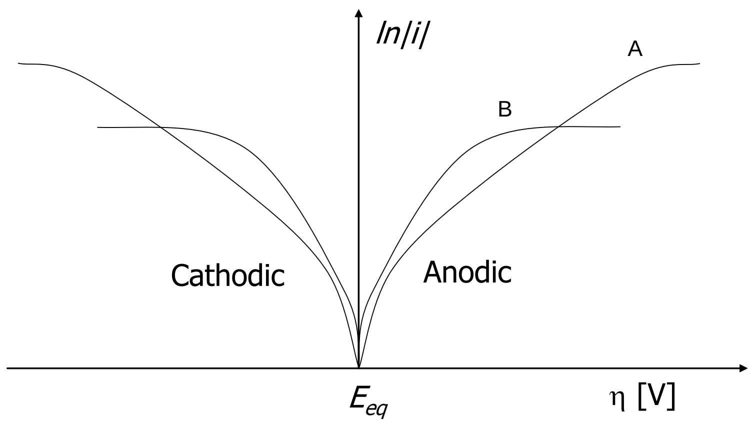
h. Give the equation for the line describing the Gibbs free energy between compositions x_1 and x_2.
i. Derive an expression in terms of G_1, G_2, x_1, and x_2 for the open cell potential between x_1 and x_2 given that $V_{OCP}=-\mu/F$.

Question 6.

a. What process in an electrochemical cell is referred to as "charge transfer".
b. If the equilibrium potential of a battery is 3 Volts, what would you expect for the potential during fast discharge? And what during fast charge? Explain your answer.

In the figure below two Tafel-plots are shown, A and B, representing two batteries.

c. Discuss the difference in behaviour between the batteries at small and large overpotentials.
d. If battery B would be a Li-ion battery, give a suggestion on how to improve battery B at high overpotentials, explain your answer.



Question 7.

a. Sketch how a modern electrolyser for the production of hydrogen from fresh water operates.
b. What efficiency can be reached for an electrolyser and what is the main loss of efficiency?
c. What do you expect to be an important cost factor for the price of an electrolyser.
d. What main impurity will be present in the hydrogen produced by electrolysis of fresh water. How would you purify the hydrogen gas taking out this main impurity efficiently? Is the impurity a problem for use in fuelcells?
e. If sea water is used what needs to be modified and why? Is this a fully established technique?

Question 8.

Solar ray to hydrogen conversion can be accomplished in various ways: solar cells combined with electrolysis, direct photocatalytic water splitting, by concentrated solar heat and by producing biomass.

a. Which of these methods is currently most energy efficient in converting solar energy into hydrogen?
b. How does the concentrated solar heat production method for hydrogen work. Name one important technological development which needs to be realized.
c. Discuss advantages and disadvantages of the use of biomass for hydrogen production.

Question 9.

a. Describe H_2 production from fossil fuels. Is this an energy efficient process?
b. Where is a catalyst needed, and where play possible unwanted side-reactions a role?

Question 10.

The clathrate hydrate consisting of water and the organic molecule THF can store hydrogen up to <1 wt.%.

a. What type of interaction is responsible for the hydrogen uptake under an applied pressure?

b. Why is the THF quoted as stabilizing the hydrogen containing clathrate?
c. At low temperature the hydrogen is trapped in the structure, but not at >220K. Why?
d. Could it be advantageous for the storage capacity to have much larger pores available for the hydrogen to sit in?

Question 11.

a. The graph below shows the pressure – composition plot of the (catalyzed) hydrogen storage material $NaAlH_4$. What kind of information can you deduce from the graph about the hydrogen desorption and absorption?
b. Estimate an enthalpy of formation from the reaction taking place at H/Al =1.8.
c. Ti based catalysts are used to catalyze reversible H uptake and release in $NaAlH_4$. Can you explain which role this catalyst plays and how?