Sustainable Hydrogen and Electrical Energy Storage, SET3031 Exam 28 June 2010

Question 1.

a. Why, and at which scale, is energy storage required in a renewable energy future?

- b. Why is hydrogen interesting as a future energy carrier? (name 5 reasons)
- c. What are the main current applications of hydrogen?

d. Is there a trend in the ratio H/C in fuels that mankind used in history? If yes, which? e. How does an oil company look at future fuel development and realizing the hydrogen economy?

Question 2.

Quantum mechanics plays a role in various aspects for hydrogen storage

a. Which quantum phenomenon plays a role with storage of liquid hydrogen, and how is this handled when liquefying hydrogen?

b. Which quantization plays a role when compressing hydrogen gas, and why is this less of a factor for propane?

c. Which valence does hydrogen normally take in metal hydrides? And in acids?

Question 3.

a. Describe the mechanism of the pressure sweep adsorption method for the purification of hydrogen.

b. Currently high purity levels are required for hydrogen, why is that? Do these requirements change when water electrolysis is used in the future?

c. What is the advantage of a Pd filter for hydrogen? How do polymeric hydrogen filters compare?

Question 4.

Consider the Daniel element with the two half reactions $Cu^{2+}(aq) + 2e^{-} > Cu(s)$ (standard potential +0.337 V) and $Zn^{2+}(aq)+2e^{-} > Zn(s)$ (standard potential -0.76 V). However, part of the Zn electrode contains Fe (Fe²⁺(aq) + 2e⁻ -> Fe(s) at standard potential -0.44 V).

- a. What will happen when the Zn + Fe electrode will be immersed in the electrolyte (containing Zn²⁺ ions)?
- b. If the Fe oxidation is much faster than the Zn oxidation, write down the half cell reactions, and determine the cell potential under standard conditions.

Now assume all Fe has been reacted and only Zn and Cu can react. Assume the starting concentrations are $c_{Cu2+}=0.1$, $c_{Zn2+}=1$ mol/liter and $c_{Cu(s)}=c_{Zn(s)}=1$. Nernst law: (Nernst: $\epsilon = (\phi_C - \phi_A) = \epsilon^O - (RT/zF)$ [In Πc_i^{v}], for example applied to the half reaction

 $Zn^{2+}(aq)+2e^{-} \rightarrow Zn(s)$ leads to $\varepsilon = \varepsilon^{O} - (RT/zF) \ln(c_{Zn(s)}/c_{Zn2+})$. R=8.31 J/(mol K), T=293 K.

- c. Calculate the open cell potential between the two electrodes under the given conditions.
- d. How much chemical energy is converted to electrical energy per mole reacted Cu(s) (Δ G=-(φ _C- φ _A)zF, F=96500 C/mol)?
- e. How can the amount of chemical energy that this cell delivers be increased without increasing the size of the Zn and Cu electrode?

f. What is the electrochemical layer, and how does it develop? Explain using the example of immersing a Zn electrode in a solution.

Question 5

- a. Sketch a Li-ion battery, explain how a Li-ion battery works, what are the components, and what is their function?
- b. For what reasons would Li-metal in principle be the ideal anode, and for what reason is it potentially unsafe?
- c. Explain what is meant by mechanical failure of Li-ion electrode materials, and what is the origin of mechanical failure.
- d. What is the main reason that Li-ion batteries have a higher energy density compared to NiMH batteries.
- e. In the figure below you see the voltage during charge and during discharge at different rates given in Ampere. Which curves are during charge en which during discharge? Why is there a difference between the voltages at different (dis)charge rates?



- f. Assume that the voltage curve at a current of 20 Ampere is on average at 1.5 V and the maximum capacity 8 Ah. Also assume that the reversible voltage is 2.35 V and that the theoretical capacity is 10 Ah. What is the theoretical energy capacity of this battery, and what is the efficiency at 20 Ampere?
- g. What may cause the internal resistance in a Li-ion battery?

Question 6

a. What is the meaning of the exchange current density I_0 ?

Below you see a Tafel plot of the two reactions that occur in a NiMH battery.



- b. In the figure above there are two ways to see that one of the electrodes is more sluggish (slower reaction rate). Which electrode is it, and what are the two ways?
- c. What process is most likely responsible for the sluggish reaction? Choose between charge transfer/ionic transport/electronic transport, and explain why.
- d. Assume we are charging the NiMH battery with a certain current. Explain how this figure can be used to determine the voltage necessary to charge the battery with this current.
- e. What is the risk if the overpotential becomes too large?

Question 7

a. Which main factors determine the equilibrium operating temperature and pressure of a hydrogen storage material? Is this equilibrium always reached?

b. For bulk magnesium hydride a van 't Hoff plot as indicated in the figure (line) can be measured. For a certain catalyzed and nanostructured magnesium hydride a somewhat different graph is measured (dashed line). Interpret the difference using what you know from catalyzed magnesium hydride.



Question 8

Ammonia as hydrogen storage material.

a. Name 3 advantages of ammonia as hydrogen storage material.

b. Name disadvantages of ammonia as storage material.

c. Why are salts attractive for binding the ammonia? What can you say about the enthalpy of formation of the ammonia, such salts, and the energy content of hydrogen that should be released from it for use as fuel?

Question 9

What main strategies are available for making the enthalpy of formation of metal hydrides less negative? Is there also a disadvantage or difficulty for these approaches?

Question 10

a. Describe the hydrogen (and oxygen) production by direct photo catalysis.
b. How does the theoretical efficiency compare to what can be realized in theory using solar cells and electrolysis (rough estimate).

c. Which criteria should the semiconductor surface that is used satisfy?