MMME2045 Functional Materials

Question 1

The $LiCoO_2$–based lithium ion batteries were first commercialised in 1991. The two half and total cell reactions during discharge are:

Electrode 1: $Li_xC_6 \rightarrow xLi^+ + 6C + xe^-$

Electrode 2: $Li_{1-x}CoO_2 + xLi^+ + xe^- \rightarrow LiCoO_2$

Overall cell reaction: $Li_{1-x}CoO_2 + Li_xC_6 \rightarrow LiCoO_2 + 6C$

The sum of the molecular weight of the reactants is 170 g mol^{-1}. The cell potential is 3.6 V. Calculate the theoretical specific capacity (express in mAh/g) and specific energy (express in Wh/kg) for the lithium ion battery (considering the mass of reactants only).

Question 2

A commercial electric car is powered by a 42-kWh lithium ion battery pack with a mass of 270 kg.

A commercial lead-acid SLI (Starting Lighting Ignition) battery has a nominal capacity of 24 Ah and voltage of 12 V. It weighs 9 kg.

If we use the lead-acid battery to store the 42-kWh electricity, calculate the mass of the lead-acid battery.

Question 3

Proton exchange membrane fuel cells (PEMFCs) can convert hydrogen into electricity directly through the electrochemical reactions below:

Electrode 1: $H_2 \rightarrow 2H^+ + 2e^-$ (1)

Electrode 2: $1/2O_2 + 2H^+ + 2e^- \rightarrow H_2O$ (2)

The overall reaction: $H_2 + 1/2O_2 \rightarrow H_2O$ (3)

Identify which electrode is the anode (negative electrode) and which electrode is the cathode (positive electrode).

The change in enthalpy (ΔH) and Gibbs free energy (ΔG) at 25 °C and 80 °C under standard pressure (1 atm) for the above reaction (3) are given in the Table below. Calculate the theoretical maximum efficiency at 25 °C and 80 °C of the above PEMFC.

	Enthalpy (ΔH, kJ/mol)	Gibbs free energy (ΔG, kJ/mol)
25 °C	-285.83	-237.13
80 °C	-281.68	-228.20

Question 4

The Table 1 below list the specifications of four commercial supercapacitors.

Product & Spec.

Rated Capacitance	Internal Resistance (mΩ)		Max. Current (A)	Leakage Current (mA)	Stored Energy (Wh)	Specific Energy (Wh/kg)	Weight (g)
Discharge with constant current at 25℃	AC(100Hz)	DC	1 sec discharge rate to $1/2V_R$	72hours, 25℃	at V_R	Gravimetric	
600F	< 0.64	< 0.83	541	1.7	0.608	2.90	210
1700F	< 0.50	< 0.65	1,090	2.4	1.721	4.47	385
3500F	< 0.28	< 0.36	2,091	5.5	3.544	5.17	685
5000F	< 0.25	< 0.33	2,547	8.1	5.063	5.44	930

Rated Voltage, V_R	2.7 V	

Calculate the stored energy and specific energy for the commercial supercapacitors.

Solutions:

Solution 1

1 Ah = 1 Amp*hour = 1 C/s * 3,600 s = 3,600 C

1 Wh = 1 J/s * 3,600 s = 3,600 J

Specific capacity = $\frac{nF}{[3600\ C/Ah*MW]} = \frac{1*96485\ C/mol}{[3600\ C/Ah * 170\ g/mol]}$

=0.158 Ah/g = 158 mAh/g

Specific energy = $\frac{nFE}{[3600\ J/Wh*MW]} = \frac{1*96485\ C/mol * 3.6\ V}{[3600\ J/Wh * 170\ g/mol]}$

=0.568 Wh/g = 568 Wh/kg

Solution 2

The specific energy of the lead acid battery

= 24 Ah × 12 V / 9 kg = 32 Wh/kg

The mass of the lead acid battery required to store the 42 kWh electricity

= 42 × 1,000 Wh / 32 Wh/kg

= 1312.5 kg.

Solution 3

Electrode 1 is the anode (negative electrode) as the oxidation reaction occurs and negatively-charged electrons are produced. Electrode 2 is the cathode (positive electrode) as the reduction reaction occurs and the negatively charged electrons move towards to this electrode.

At 25 °C, the theoretical efficiency

$\eta = \Delta G / \Delta H$ = (-237.13 kJ/mol) / (-285.83 kJ/mol) = 83%

At 80 °C, the theoretical efficiency

$\eta = \Delta G / \Delta H$ = (-228.20 kJ/mol) / (-281.68 kJ/mol) = 81%

Solution 4

Stored energy $E = \frac{1}{2} CU^2$

From the Table, $U = 2.7$ V.

C =600 F

$E = \frac{1}{2} \times 600 \text{ F} \times 2.7 \text{ V} \times 2.7 \text{ V} = 2187 \text{ J} = 2187 \text{ J} / (3600 \text{ J Wh}^{-1}) = 0.608 \text{ Wh}$

Specific energy = 0.608 Wh / 0.210 kg = 2.90 Wh/kg

C =1700 F

$E = \frac{1}{2} \times 1700 \text{ F} \times 2.7 \text{ V} \times 2.7 \text{ V} = 6197 \text{ J} = 6197 \text{ J} / (3600 \text{ J Wh}^{-1}) = 1.721 \text{ Wh}$

Specific energy = 1.721 Wh / 0.385 kg = 4.47 Wh/kg

C =3500 F

$E = \frac{1}{2} \times 3500 \text{ F} \times 2.7 \text{ V} \times 2.7 \text{ V} = 12758 \text{ J} = 12758 \text{ J} / (3600 \text{ J Wh}^{-1}) = 3.544 \text{ Wh}$

Specific energy = 3.544 Wh / 0.685 kg = 5.17 Wh/kg

C =5000 F

$E = \frac{1}{2} \times 5000 \text{ F} \times 2.7 \text{ V} \times 2.7 \text{ V} = 18225 \text{ J} = 18225 \text{ J} / (3600 \text{ J Wh}^{-1}) = 5.063 \text{ Wh}$

Specific energy = 5.063 Wh / 0.930 kg = 5.44 Wh/kg