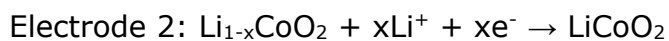
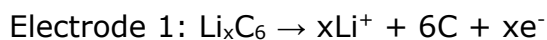


MMME2045 Functional Materials

Question 1

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



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

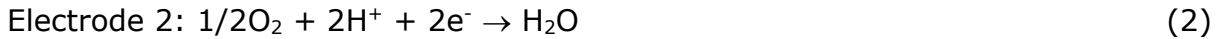
A commercial electric car is powered by a 42-kWh lithium ion battery pack with a mass of 270 kg.

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:



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 (m Ω)		Max. Current (A)	Leakage Current (mA)	Stored Energy (Wh)	Specific Energy (Wh/kg)	Weight (g)
	Discharge with constant current at 25°C	AC(100Hz)	DC	1 sec discharge rate to 1/2V _R	72hours, 25°C	at V _R	
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

$$1 \text{ Ah} = 1 \text{ Amp} \cdot \text{hour} = 1 \text{ C/s} \cdot 3,600 \text{ s} = 3,600 \text{ C}$$

$$1 \text{ Wh} = 1 \text{ J/s} \cdot 3,600 \text{ s} = 3,600 \text{ J}$$

$$\begin{aligned} \text{Specific capacity} &= \frac{nF}{[3600 \text{ C/Ah} \cdot \text{MW}]} = \frac{1 \cdot 96485 \text{ C/mol}}{[3600 \text{ C/Ah} \cdot 170 \text{ g/mol}]} \\ &= 0.158 \text{ Ah/g} = 158 \text{ mAh/g} \end{aligned}$$

$$\begin{aligned} \text{Specific energy} &= \frac{nFE}{[3600 \text{ J/Wh} \cdot \text{MW}]} = \frac{1 \cdot 96485 \text{ C/mol} \cdot 3.6 \text{ V}}{[3600 \text{ J/Wh} \cdot 170 \text{ g/mol}]} \\ &= 0.568 \text{ Wh/g} = 568 \text{ Wh/kg} \end{aligned}$$

Solution 2

The specific energy of the lead acid battery

$$= 24 \text{ Ah} \times 12 \text{ V} / 9 \text{ kg} = 32 \text{ Wh/kg}$$

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

$$= 42 \times 1,000 \text{ Wh} / 32 \text{ Wh/kg}$$

$$= 1312.5 \text{ kg.}$$

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

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

At 80 °C, the theoretical efficiency

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

Solution 4

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

From the Table, $U = 2.7 \text{ V}$.

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 = $0.608 \text{ Wh} / 0.210 \text{ kg} = 2.90 \text{ Wh/kg}$

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 = $1.721 \text{ Wh} / 0.385 \text{ kg} = 4.47 \text{ Wh/kg}$

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 = $3.544 \text{ Wh} / 0.685 \text{ kg} = 5.17 \text{ Wh/kg}$

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 = $5.063 \text{ Wh} / 0.930 \text{ kg} = 5.44 \text{ Wh/kg}$