23CGP070

Clean Energy, Materials and Sustainability

Semester 2 2023/24 | In-Person Exam paper

This examination is to take place in-person at a central University venue under exam conditions. The standard length of time for this paper is **3 hours**.

You will not be able to leave the exam hall for the first 30 or final 15 minutes of your exam. Your invigilator will collect your exam paper when you have finished.

<u>Help during the exam</u>

Invigilators are not able to answer queries about the content of your exam paper. Instead, please make a note of your query in your answer script to be considered during the marking process.

If you feel unwell, please raise your hand so that an invigilator can assist you.

You may use a calculator for this exam. It must comply with the University's Calculator Policy for In-Person exams, in particular that it must not be able to transmit or receive information (e.g., mobile devices and smart watches are **not** allowed).

Attempt **ALL** questions. Each question carries 25 marks.

Candidates should show full working for all calculations and derivations.

An Appendix of constants and conversions is available on the final page of the exam paper.

1. (a) For a proton-exchange-membrane fuel cell (PEMFC) running at 60°C and an alkaline fuel cell (AFC) running at 70°C, hydrogen gas is feeding to anodes, and air is feeding to cathodes. Write and balance the anode half-cell reaction, the cathode half-cell reaction, and the full-cell reaction of these two fuel cells (PEMFC and AFC). Specify the states (gas, liquid or solid) of all reactants and products in these reactions. [6 marks]

   (b) Comparing the two fuel cells in 1(a) (the PEMFC running at 60°C and the AFC running at 70 °C), which one has a higher *reversible thermodynamic efficiency*? Briefly justify your answer. [4 marks]

   (c) A solid oxide fuel cell (SOFC) uses methane (CH_4) gas as the fuel in the anode feed and oxygen gas as oxidant in the cathode feed. Assuming the SOFC operates at 727°C, write and balance the anode half-cell reaction, the cathode half-cell reaction, and the full-cell reaction. [3 marks]

   (d) Given the thermodynamic data in **Table Q1**, and assuming that both the enthalpy and entropy are independent of temperature, calculate the *reversible thermodynamic efficiency* of a methane-oxygen solid oxide fuel cell running at 727°C. [4 marks]

   (e) If this solid oxide fuel cell is supplied with 1 bar methane at the anode and 1 bar oxygen at the cathode, calculate the *reversible cell potential* (E^o) at 727°C. [3 marks]

   (f) If this methane-oxygen solid oxide fuel cell generates 500 A at an overvoltage loss of 0.10 V at 727°C, calculate the *real efficiency* of this fuel cell. Methane and oxygen are supplied to the fuel cell at 0.001 mol s^{-1} and 0.002 mol s^{-1}; respectively. [5 marks]

Table Q1. Thermodynamic Data

Chemical Species	$\mathbf{D}\hat{h}_f^0$ **(kJ mol^{-1})**	$\mathbf{D}\hat{s}^0$ **(J mol^{-1} K^{-1})**
CH_4 (g)	-74.80	186.25
O_2 (g)	0	205.00
CO_2 (g)	-393.51	213.79
H_2O (g)	-241.83	188.84

2. (a) A 16 cm^2 proton-exchange membrane fuel cell has the electronic resistance of 0.001 Ω and the electrolyte ionic conductivity of 0.100 Ω^{-1} cm^{-1}. If the electrolyte is 40 μm (micro-meter) thick, calculate the ohmic voltage loss for this fuel cell running at a current density of 800 mA cm^{-2}. [5 marks]

(b) In the following electrochemical cell at 298 K shown in the shorthand expression (cell notation) below, write down and balance the oxidation half-cell reaction, the reduction half-cell reaction, and the full-cell reaction. Calculate the electromotive force (EMF) of this cell. Standard Redox Potentials data are shown in **Table Q2** that you can choose to use as appropriate. [9 marks]

Cu^{2+}(aq, 0.001M) │ Cu(s) ‖ H^+(aq, 0.1M) │ H_2(g, 1 atm)

Table Q2. Standard Potentials at 298 K.

Half-cell reaction	E^0 (V)
$Cu^{2+}(aq) + 2e^- \rightarrow Cu(s)$	0.34
$2H^+(aq) + 2e^- \rightarrow H_2(g)$	0.00

(c) A computer requires the voltage of 6.00 V and the current of 10.00 A to power it.

(i) If a single proton-exchange-membrane fuel cell can deliver a current of 5.00 A at the voltage of 0.60 V, how many of the single fuel cells are required and how do they need to be arranged together to power this computer? Briefly justify your answer. [3 marks]

(ii) This computer needs to be operated for 200 hours. Assuming 70% real efficiency of the fuel cells, what is the minimum amount of hydrogen gas (H_2) fuel (in moles) required? [6 marks]

(iii) If methanol (CH_3OH) fuel is used to replace H_2 in (ii), with all other conditions being the same, what is the minimum amount of methanol fuel (in moles) required? [2 marks]

3. (a) Briefly explain how changes in the grain size could impact the hydrogen storage performance of MgH_2. [4 marks]

(b) Discuss the mechanism of the "nanopump effect" that has been proposed as a responsible phenomenon for improved hydrogen storage in 2D materials such as stacked graphene. [6 marks]

(c) Figure Q3 shows discharge curves of crystalline and amorphous V_2O_5 in a sodium-ion battery. Discuss the effect of the degree of crystallinity on the performance of V_2O_5 as an electrode material in this battery system. [3 marks]

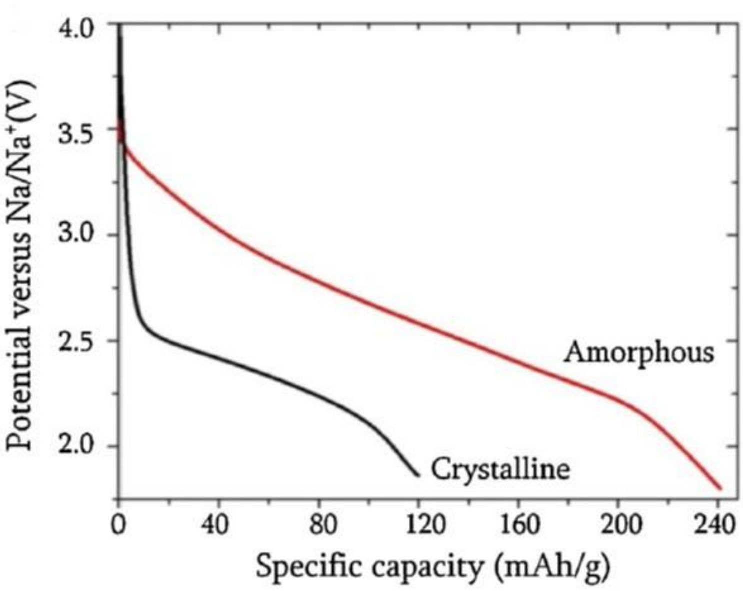

Figure Q3

(d) State TWO of the main consequences of formation of Li dendrites in Li-ion batteries and explain the governing mechanisms responsible for the growth of this morphology. [8 marks]

(e) Propose TWO approaches to improve the energy density of a Li ion battery. Your answer should provide a justification for the validity of the proposed solution. [4 marks]

4. (a) A lithium-ion battery cell has been manufactured using a graphite host C_6Li and $LiCoO_2$ as negative and positive electrodes, respectively.

   (i) Provide the overall electrochemical reaction for the battery. [1 mark]

   (ii) Calculate the theoretical specific capacity for the two electrodes in mAh g^{-1}. [2 marks]

   (iii) Calculate the gravimetric energy density of the battery system in terms of Wh kg^{-1} operating at an Open Circuit Voltage (OCV) of 2.1 V. [2 marks]

Assume the following atomic mass (in amu) values for the different elements: Li:7, C:12, Co:59, O:16.

$$C_{max} = \frac{nF}{3.6\ M_w} \quad [mAh\ g^{-1}]$$

$$F = 96500$$

(b) One of the most effective approaches to develop more sustainable technologies is to implement the 12 Green Engineering Principles. Principle 3 is “design for separation”.

   (i) Elaborate the meaning of this principle. [2 marks]

   (ii) Give a specific engineering example and use the example to explain in detail how the principle is implemented in real world. [1 mark]

(c) (i) What is Atom Economy? [1 mark]

   (ii) Please calculate the Atom Economy of (A) ammonia synthesis from the Haber–Bosch process with the reaction of $N_2(g) + 3H_2(g) \rightarrow 2NH_3(g)$ and (B) methanol synthesis from carbon monoxide and hydrogen with the reaction of $CO(g) + 2H_2(g) \rightarrow CH_3OH(l)$. [4 marks]

   (iii) Compare the values of Atom economy from the two reactions in (ii), and what is the indication from different values of atom economy? [2 marks]

Data: Molecular weight of

N_2: 28 g/mol, H_2: 2 g/mol, NH_3: 17 g/mol, CO: 28 g/mol, CH_3OH: 32 g/mol

Continued/…

Q4 Continued/…

(iv) A 2000 MWe natural gas power plant is operating continuously over the year on a 60% energy efficiency. The associated CO_2 emission is 0.05 kg per kWhe. A carbon capture process is to be installed on this power plant. The Carbon CaptureS unit can capture 78% of the CO_2 in the exhaust while the energy penalty is 12%.

(a) How much CO_2 emission can be saved annually? [7 marks]

(b) What is the value of Effective CO_2 Capture Fraction? [3 marks]

END OF PAPER

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APPENDIX
CONSTANTS AND CONVERSIONS

Physical Constants		
Avogadro's number	N_A	6.02×10^{23} atoms/mol
Universal gas constant	R	$0.08205\ L \cdot atm/mol \cdot K$
		$8.314\ J/mol \cdot K$
		$83.14\ bars \cdot cm^3/mol \cdot K$
		$8.314\ Pa \cdot m^3/mol \cdot K$
Planck's constant	h	$6.626 \times 10^{-34}\ J \cdot s$
		$4.136 \times 10^{-15}\ eV \cdot s$
Boltzmann's constant	k	$1.38 \times 10^{-23}\ J/K$
		$8.61 \times 10^{-5}\ eV/K$
Electron mass	m_e	9.11×10^{-31} kg
Electron charge	q	1.60×10^{-19} C
Faraday's constant	F	96485.34 C/mol

Conversions	
Weight	2.20 lb = 1 kg
Distance	0.622 mile = 1 km
	3.28×10^{-2} ft = 1 cm
Volume	1000 L = 1 m^3
	0.264 gal = 1 L
	$3.53 \times 10^{-2}\ ft^3$ = 1 L

Conversions (cont.)	
Pressure	1.013250×10^5 Pa = 1 atm
	1.013250 bars = 1 atm
	10^5 Pa = 1 bar
	14.7 psi = 1 atm
Energy	6.241506×10^{18} eV = 1 J
	1 calorie = 4.184 J
	9.478134×10^{-4} Btu = 1 J
	2.777778×10^{-7} kWh = 1 J
Power	1 J/s = 1 W
	$1.34 \cdot 10^{-3}$ horsepower = 1 W
	3.415 Btu/h = 1 W