

國立臺灣科技大學102學年度碩士班招生試題

系所組別：材料科學與工程系碩士班甲組

科目：物理化學

(總分為100分)

總分 100 分，共 8 大題。

Useful physical constants:

Planck constant(h)= 6.626×10^{-34} J-s ; $h/(2\pi) = 1.05 \times 10^{-34}$ J-s ;Electron mass= 9.1×10^{-31} kg ; Electron charge= 1.6×10^{-19} C

1. (10 points) Copper has lattice constant (a)= 0.36153 nm, mass density= 8.92×10^6 g/m³, and atomic mass= 63.546 g/mol. It is analyzed with an X-ray diffractometer.
- 1) Show that the atomic arrangement is face-centered cubic (F.C.C.), with given data. (5 points)
 - 2) What's the angle between the incident X-ray (wavelength= 0.1542 nm) beam and (200) crystal plane. (5 points)

2. (10 points) For a reaction $A + B \rightarrow Z$ with a mechanism:



- 1) Write differential rate equations for species A, B, X, and Z. (4 points)
 - 2) Define the reaction rate as the formation rate of product Z. While the concentration of X is small, there is consequently a steady state for X. Present the reaction rate as a function of reactant concentrations. (3 points)
 - 3) While k_2 is much greater than k_{-1} , try to simplify the equation obtained from the above question, and write the single rate-controlling step in the mechanism. (3 points)
3. (10 points) For an electron in 3d orbitals of a hydrogenlike atom,
- 1) Give the orbital angular momentum of an electron. (2 pt)
 - 2) Give the possible values of z component of orbital angular momentum. (3 pt)
 - 3) Give the possible values of z component of magnetic dipole moment. (3 pt)
 - 4) Give the total spin angular momentum. (2 pt)
4. (10 points) An electron has a kinetic energy of 1.602×10^{-17} J,
- 1) Find the momentum of an electron. (3 pt)
 - 2) Find the wavelength of an electron. What's the wavenumber? (4 pt)
 - 3) If the uncertainty in the position of the electron is 1 nm, use the Heisenberg uncertainty principle to find the uncertainty of momentum. (3 pt)



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5. (10 points) Given the wavefunction for 1s electron in hydrogenlike atom (atomic number = Z):

$$\Psi = \pi^{-1/2} (Z/a_0)^{3/2} \exp(-Zr/a_0)$$

where r is distance between the nucleus and electron.

- 1) Give the physical meaning of a_0 in the above expression. What is its numerical value? (3 pt)
 - 2) Define radial probability density, and find the probability for the electron appearing between $r = 0.5a_0$ and $r = 0.6a_0$. (Note: You don't need to evaluate the value of integral.) (4 pt)
 - 3) The ionization energy of hydrogen is 13.6 eV. What's the binding energy for the electron in Li^{2+} ion? (Z of Li atom = 3) (3 pt)
6. The van der Waals equation is common used to describe the real gas behavior. For one mole of gas, it is written as

$$(P + a/V^2)(V - b) = RT$$

Where P is the measured pressure of the gas, a/V^2 is a correction term for the interactions which occur among the particles of the gas, V is the measured volume of the gas, and b is a correction term for the finite volume of the particles. Please show the "a" and "b" with critical properties of the gas in the van der Waals equation. Where T_{cr} , P_{cr} and V_{cr} are the critical temperature, pressure and volume of the gas. (15 points)

7. (a) What is the Giggis-Duhem (G-D) equation? (5 points)

(b) Use the G-D equation, please show the following equations,

$$\bar{M}_1 = M + x_2 \frac{dM}{dx_1}$$

$$\bar{M}_2 = M - x_1 \frac{dM}{dx_1}, \text{ where the } \bar{M}_1 \text{ \& } \bar{M}_2 \text{ are the partial properties of } M_1 \text{ and } M_2.$$

M can be expressed as G , H and V .

(15 points)

8. Explain the following terms:

- (a) Phase Rule. (5 points)
- (b) First Law of Thermodynamics. (5 points)
- (c) excess property. (5 points)

