CHEM2100J Chapter 00-02 RC

CHEM2100J Teaching Team
UM-SJTU Joint Institute
elysia-ego@sjtu.edu.cn
October 8, 2023

Contents

Introduction----Homework,quizzes and exams

- Homework

  Help you prepare for quizzes, exams.

  Receive 0 after the due date.

  Only contains multiple choice questions, only retains the last attempt

- Quizzes

  the questions will be different between individuals.

  short examinations of 10 min length on a regular basis,

- Exams

  A 45 minutes midterm exam and a 100 minutes final exam

  No dictionaries.

  Prepare your cheating paper!

Introduction----advice

- Attend and listen carefully in lectures and RC.
- Practice your skills on using calculator.
- Carefully finish the homework; refer to exercises in the textbook if you have time.
- Read Chemical Principle before and after the lectures. Don’t rely too much on Chinese textbooks.
- Ask questions at OH as much as possible. TAs reserve the rights not to answer questions asked via WeChat and Feishu.

Fundamentals---significant figures

- **Counting rule**

  Count the number of figures starting from the first non-zero one.

Number	# of significant digits	Rule
7,813	4	All digits 1–9 count
600.3	4	Captive count
0.00002	1	Leading never count
9.800	4	Trailing with decimal count
504.010	6	Captive and trailing with decimal count
4,000,000	1	Trailing without a decimal never count
5.00×10^6	3	Scientific notation only display SF

Fundamentals---significant figures

- Examples:

• 1.070	4
• 0.0028	2
• 100	1
• 100.	3
• 3.14×10^{4}	3

Fundamentals---significant figures

- **Rounding rule**

Above 5 - round up

Exactly 5 - round to even if no figures behind; round up otherwise

Below 5 - round down

- **Operational rule**

+-: follow the least decimal place

*/: follow the least significant figures

exponent: decimal place of index = significant figures of answer

logarithm: significant figures of antilogarithm = decimal place of answer

- **Don't round up in the middle of the calculation!**

Fundamentals---significant figures

- Example:

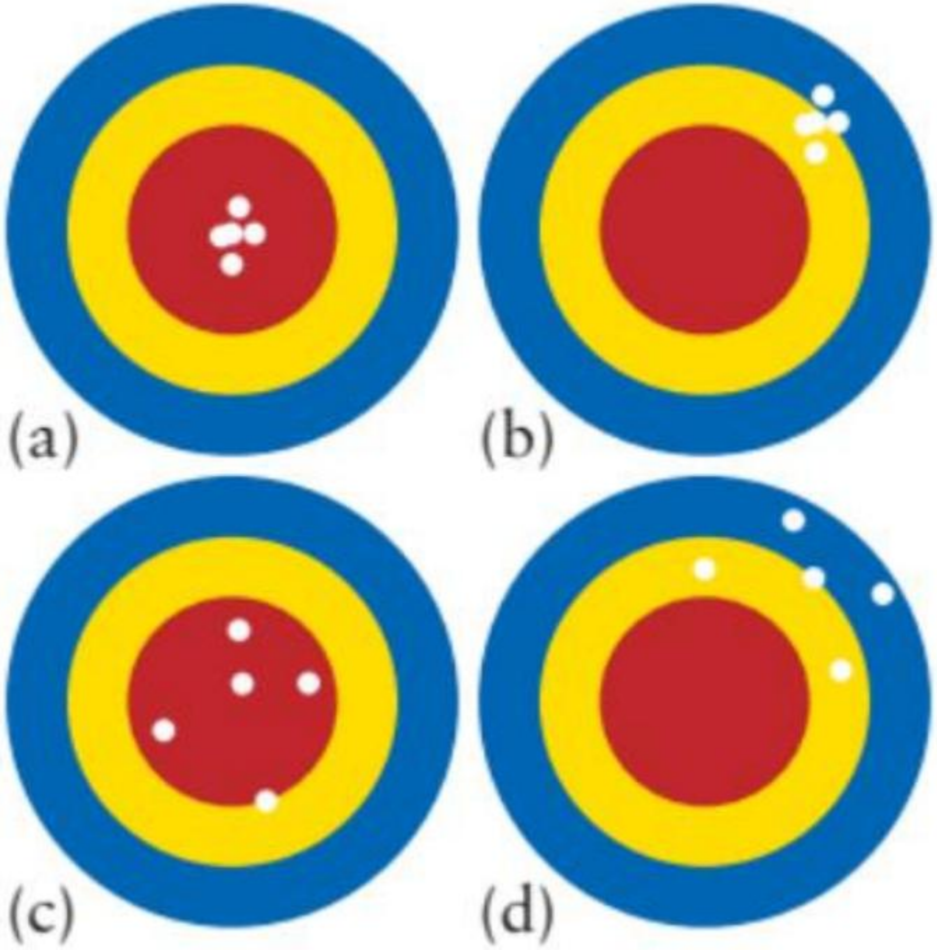
$(317.89+1.3)\times 989.46$

Determine the number of the significant figures.

- Answer: 4

fundamental---accuracy

- (a):accurate & precise
- (b):precise
- (c):accurate
- (d):neither accurate nor precise



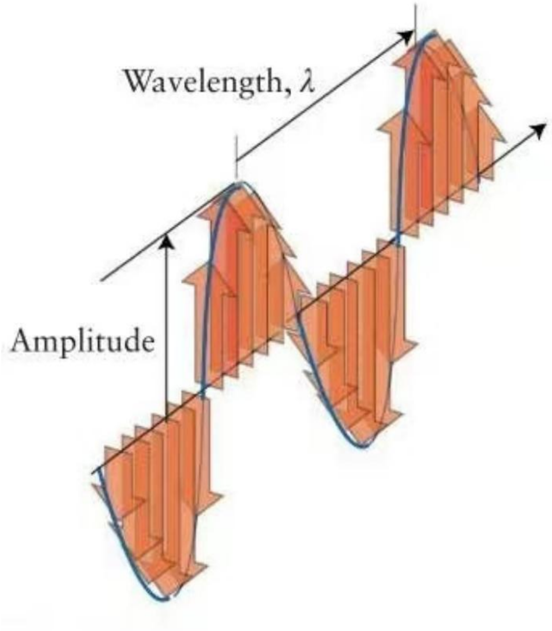
fundamentals-----property

- Extensive properties: depends on the quantity of matter
- Intensive properties: independent of the quantity of matter

- Example: determine whether extensive or intensive properties
- pressure
- volume
- density
- temperature
- speed

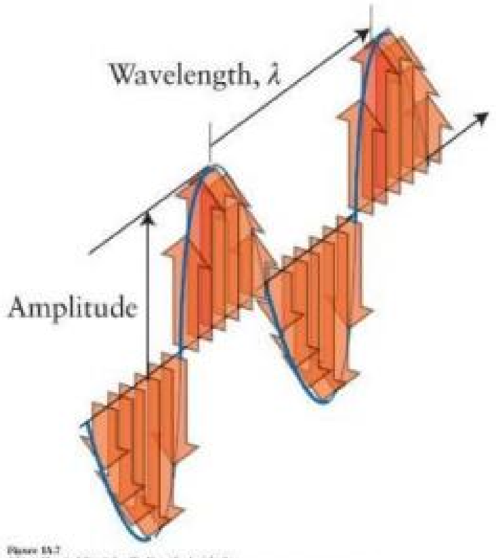
Atomic theory

- Formula: $\lambda \times \nu = c$
- Amplitude:
  - the height above the centerline
  - intensity is propotional to the amplitude squared
- Wavelength
  - distance between peaks



Atomic theory---copy it in cheating paper!

Radiation type	Frequency (10^{14} Hz)	Wavelength (nm, 2 sf)*	Energy per photon (10^{-19} J
x-rays and γ-rays	$\geq 10^3$	≤ 3	$\geq 10^3$
ultraviolet	8.6	350	5.7
visible light			
violet	7.1	420	4.7
blue	6.4	470	4.2
green	5.7	530	3.8
yellow	5.2	580	3.4
orange	4.8	620	3.2
red	4.3	700	2.8
infrared	3.0	1000	2.0
microwaves and radio waves	$\leq 10^{-3}$	$\geq 3 \times 10^6$	$\leq 10^{-3}$



Atomic theory

Democritus

Dalton

J.J.Thomson - "Plum-pudding Model"

- Cathode ray experiment
- Ratio of an electron's charge to its mass $\frac{e}{m_e}$

Millikan

- Oil drop experiment
- $e = 1.62 \times 10^{-19}\text{C},\ m_e = 9.11 \times 10^{-31}\text{kg}$

Rutherford - "Nuclear Model"

- α Scattering Experiment

Bohr - Bohr atomic model

Quantum theory

- Stefan-Boltzmann law
  - describes the exponential-like behavior of the total intensity of black body objects
  - Total intensity$=$*const* $\times\ T^4$
  - *const*$=5.67\times10^{-8}\ \mathrm{W}\cdot\mathrm{m}^{-2}\cdot\mathrm{K}^{-4}$
- Wien's law
  - shows a maximum energy density exists in black body radiation
  - $T\lambda_{max} = const$
  - *const*$=2.898\times10^{-3}$ m/K

Quantum theory

- Exercise:

Calculate the temperature of a sun whose maximum intensity of radiation occurs at 510 nm. Use 0.2898 cm/K as constant.

- Solution:

According to Wien's law, Tλmax = const, we have:

$$T = \frac{0.2898\times10^{-2}}{510\times10^{-9}}K = 5.68\times10^{4}$$

Quantum theory----Photoelectric Effect

The effect illustrates the particle nature of light.

The threshold frequency is $\nu_0 = \frac{\Phi}{h}$

$$E_{photon} = KE_{electron} + WorkFunction_{metal}$$

$$h\nu = \frac{1}{2}m_e v^2 + \Phi$$

Quantum theory----Photoelectric Effect

Exercise:

Calculate the velocity of an electron ejected from a metal with a work function of 4.28eV while being irradiated with light with a wavelength of 140 nm.

Solution:

Based on these euqations, we can find:

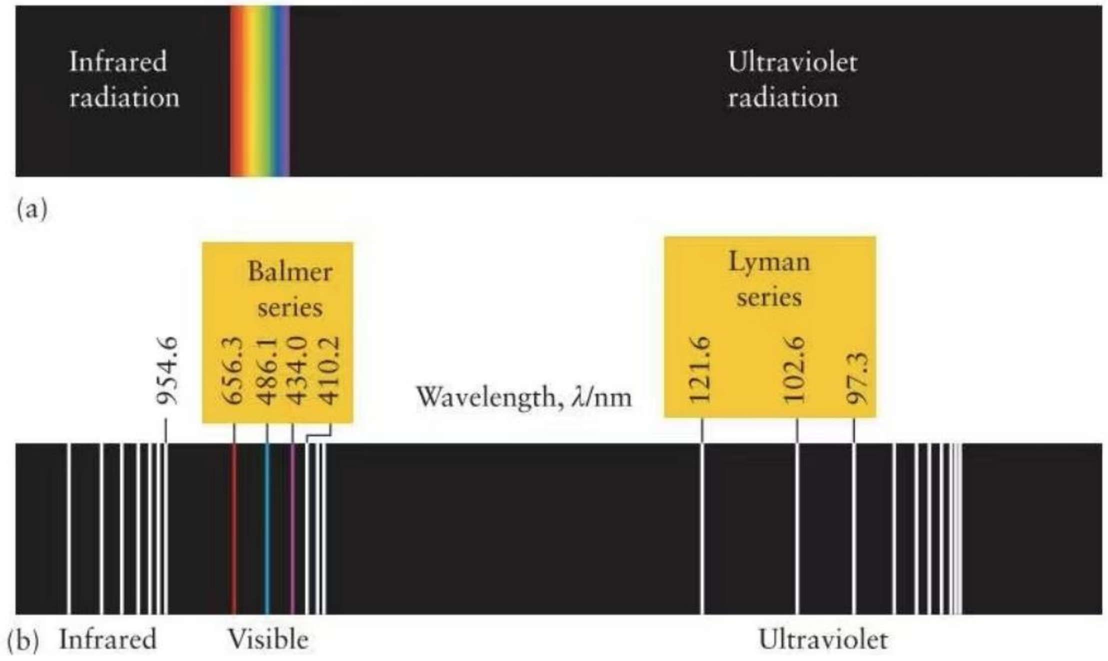
$v = 1.27 \times 10^6 m/s$

$$\frac{1}{2} m_e v^2 = h\nu - \Phi$$

$$\nu = \frac{c}{\lambda}$$

Quantum theory----Emission Spectra of Hydrogen

- **Formulas**
  - $\nu = \mathcal{R}(\frac{1}{n_1^2} - \frac{1}{n_2^2})$, $n_1 = 1, 2, ...; n_2 = n_1 + 1, n_1 + 2, ...$
  - $\frac{1}{\lambda} = \mathcal{R}_\lambda(\frac{1}{n_1^2} - \frac{1}{n_2^2})$, $n_1 = 1, 2, ...; n_2 = n_1 + 1, n_1 + 2, ...$
  - Rydberg constant: $\mathcal{R} = 3.29 \times 10^{15}\text{Hz}$, $\mathcal{R}_\lambda = 1.097 \times 10^7 m^{-1}$
- Balmer series - $n_1 = 2$, $n_2 = 3, 4...$
- Lyman series - $n_1 = 1$, $n_2 = 2, 3...$



Quantum theory----Emission Spectra of Hydrogen

Exercise

- Use the Rydberg formula for atomic hydrogen to calculate the wavelength of radiation generated by the transition from $n = 2$ to $n = 1$
- What is the name given to the spectroscopic series to which this transition belongs?
- Determine the region of the spectrum in which the transition takes place?

Quantum theory----Emission Spectra of Hydrogen

- Solution:
  - a: $\mathrm{v} = 3.29 \times 10^{15} \times (\frac{1}{1^2} - \frac{1}{2^2}) = 2.4675 \times 10^{15}$

    $$\lambda = \frac{c}{v} = \frac{3\times10^{8}}{2.4675\times10^{15}} = 1.21\times10^{-7}m$$
  - b: Lyman series
  - c: ultraviolet region

Quantum theory----Wave-Particle Duality

de Broglie relation

$$\lambda = \frac{h}{p}$$

- matter has both wavelike and particlelike properties
- matter behaves wave properties as it propagates
- matter behaves particle properties when it interacts

Quantum theory----Wave-Particle Duality

- Exercise:

The Gloriana-class battleship Hand of Dorn (m = 160 Mt) has engaged its sub-light engines and accelerated to 0.55c. Calculate the deBroglie wavelength.

- Solution:

According to de Broglie's relation,

$$\lambda = \frac{h}{p} = \frac{h}{mv} = \frac{6.626 \times 10^{-34}}{160 \times 10^{9} \times 0.55 \times 3 \times 10^{8}}\,\mathrm{m} = 2.51 \times 10^{-53}\,\mathrm{m}$$

Quantum theory----Heisenberg Uncertainty Principle

- $\Delta x \Delta p \geqslant \frac{1}{2}\hbar$
- $\hbar = \frac{h}{2\pi}$
- Δx is the uncertainty of position and Δp is the uncertainty of momentum

Quantum theory----Heisenberg Uncertainty Principle

- Exercise:

Estimate the minimum uncertainty of the position of a 2.0g marble given that its speed is known within ± 0.30 mm/s.

- Solution:

$$\Delta \mathrm{p} = \mathrm{m}\Delta \mathrm{v} \le 2.0\times 10^{-3} \times 0.6\times 10^{-3}\, kg\cdot m/s = 1.2\times 10^{-6}\, kg\cdot m/s$$

$$\Delta \mathrm{x} \ge \frac{\quad}{2\Delta p} \ge \frac{6.626\times 10^{-34}}{4\times 3.14\times 1.2\times 10^{-6}} = 4.4\times 10^{-29}\, m$$

Quantum theory---Wave Function and Schr¨odinger Equation

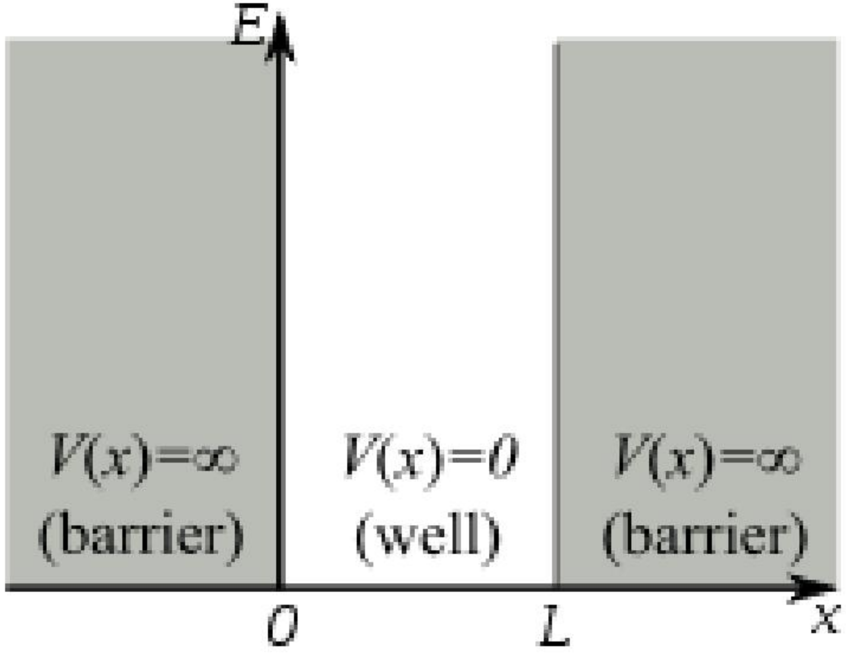
Wave function

- Ψ - describes the state of microsystem; represents AO or MO in atomic or molecular system
- Ψ^2 - represents the probability density (NOT PROBABILITY!) of electrons in atoms or molecules
- Node - the point where $\Psi = 0$(the probability of finding electrons is 0)

Schrödinger Equation

- the intrinsic form: $-\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi = E\Psi$
- $-\frac{\hbar^2}{2m}\nabla^2\Psi$ stands for the kinetic energy, $V\Psi$ stands for the potential energy and E stands for the total energy

Quantum theory-----Particle in 1D Box



Solving the Schrödinger Equation, we obtain the following results:

- when $x \leqslant 0$ or $x \geqslant L$, $\Psi(x) = 0$
- when $0 < x < L$, $\Psi_n(x) = \sqrt{\frac{2}{L}} sin(\frac{n\pi x}{L})$, n=1,2,...

Quantum theory-----Particle in 1D Box

Exercise

A particle of mass m is confined in a 1D box of length L. Given that the quantum number n, and Plank constant h is known, please verify that $E_n = \frac{n^2 h^2}{8mL^2}$.

Solution

As the wave function of the particle is $\Psi_n(x) = \sqrt{\frac{2}{L}} sin(\frac{n\pi x}{L})$, its wave length satisfies $L = n \times \frac{\lambda}{2}$, thus $\lambda = \frac{2L}{n}$. Using de Broglie's equation, we obtain that $E_n = \frac{p^2}{2m} = \frac{h^2}{2m\lambda^2} = \frac{n^2 h^2}{8mL^2}$.

Remarks:

- energy levels are quantized and determined by n
- multiple possibilities of the state of motion
- as m,L increase, the separations between energy levels decrease

Quantum Numbers, Shells and Subshells

TABLE 1D.2 Quantum Numbers for Electrons in Atoms

Name	Symbol	Values	Specifies	Indicates
principal	n	$1, 2, \ldots$	shell	size
orbital angular momentum*	l	$0, 1, \ldots, n-1$	subshell: $l = 0, 1, 2, 3, 4, \ldots$ s, p, d, f, g, ...	shape
magnetic	m_l	$l, l-1, \ldots, -l$	orbitals of subshell	orientation
spin magnetic	m_s	$+\frac{1}{2}, -\frac{1}{2}$	spin state	spin direction

Remarks:

- n,l determine the energy level of an orbital
- l,m_l determine the shape and orientation of an orbital
- m_s is independent with the other three quantum numbers

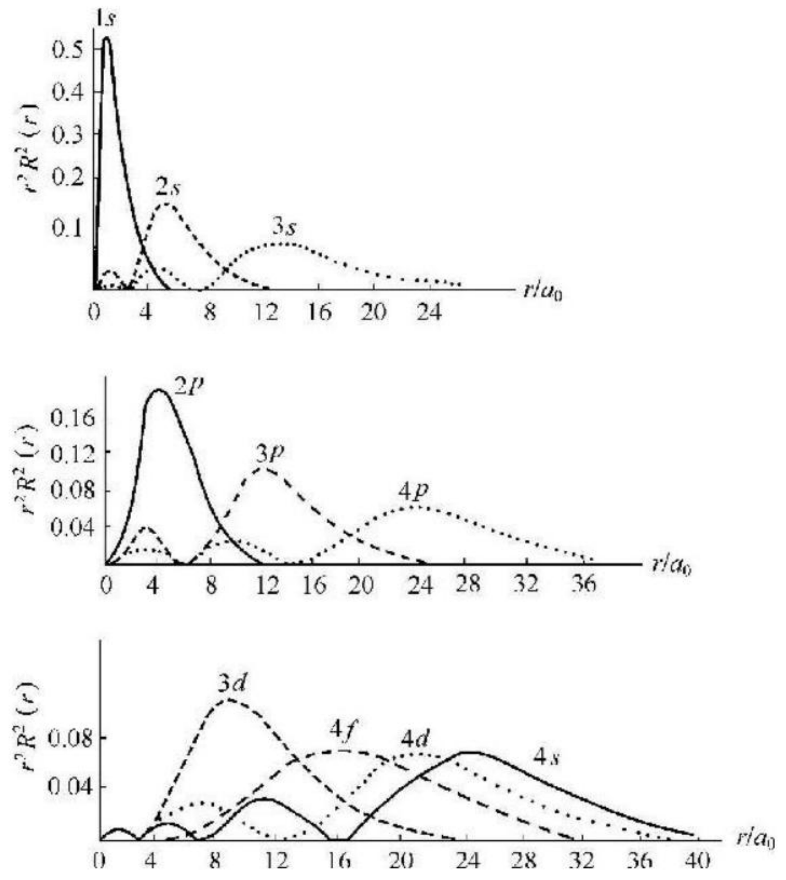
The hydrogen atom---the shape of orbitals

Shape of:

- s orbitals - sphere
- p orbitals - spindle
- d orbitals - petal

Number of:

- total orbitals$=n^2$
- total nodes$=n-1$
- radial nodes$=n-l-1$
- nodal planes$=l$



Radial distribution function of AO

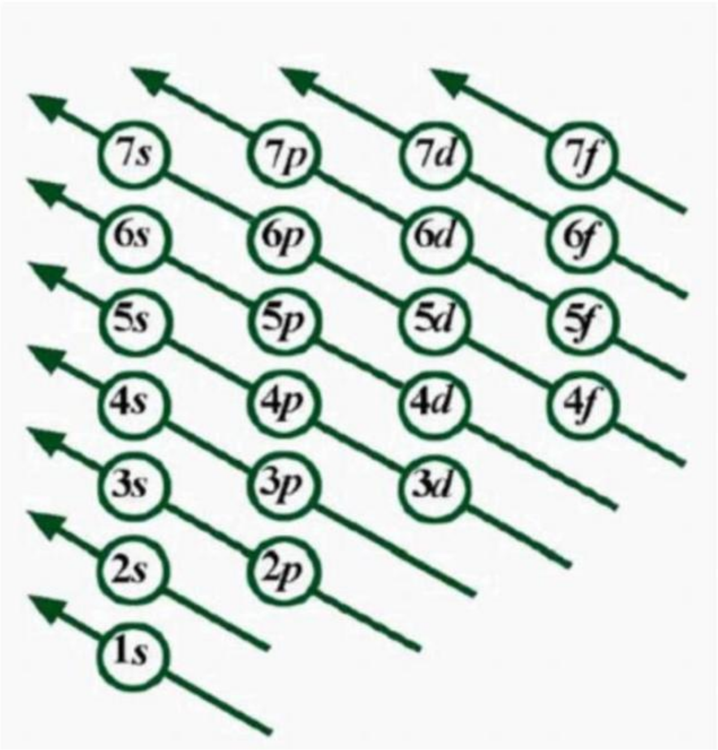
Very important

Shielding Effect & Penetration Effect

- Shielding effect
  - due to the repulsion of the electrons on inner orbitals, the outer electrons will be shielded from the full attraction of the nucleus.
  - the effective nuclear charge $Z_{eff}e$ is always less than the nuclear charge Ze
  - will cause the energy of electrons $\uparrow$
- Penetration effect
  - the electrons also have the ability to penetrate through the inner cells
  - will cause the energy of the electrons $\downarrow$

Orbital Energies

- $E_n = -\frac{Z_{eff}^2 h\mathcal{R}}{n^2}$, n=1,2,...
- In a many-electron atom, because of penetration effect and shielding effect, the order of orbital energies in a given shell is $s < p < d < f$
- Between different shells, the energy levels may overlap



The Building-Up Principle

- Pauli exclusion principle
  - No more than two electrons may occupy any given orbital
  - When two electrons do occupy one orbital, their spins must be paired($\uparrow$ and $\downarrow$)
  - In other words, no two electrons in an atom can have the same set of four quantum numbers
- Hund's rule
  - If more than one orbital in a subshell is available, add electrons with parallel spins($\uparrow\uparrow$) to different orbitals of that subshell rather than pairing two electrons in one of the orbitals (lowest total energy)
  - Exceptions: half-complete or complete subshell configuration have lower energy

Electron Configuration

- Valence shell - the occupied shell with the largest value of n
- Valence electron - the electrons in the outermost shell
- Ground state - electrons are in the lowest energy state
- Excited state - electrons are in energy states higher than the ground
- state
- Exercise: write the electron configuration
    - Fe^{2+}
    - Mn^{2+}
    - Al^{3+}
    - Zn^{2+}
    - Cu^{2+}

Reference

- Atkins, P. (2016) Chemical principles: The quest for insight. New
- York: W H Freeman.
- Prof. Milias Liu, Lecture Slides. 24FA VC210
- ZENG Haoxuan, RC Slides. 23FA VC210
- SONG Wanli, RC Slides, 23FA VC210

Thanks