1.3 Electrons, energy levels and atomic orbitals

Name: ______________ Class: __________ Date: ____________ **Total: 29 marks**

KEY WORDS electronic configuration 电子排布 • orbital 轨道 • sub-shell 亚层 • shell 壳层 • proton number 质子数

Objective

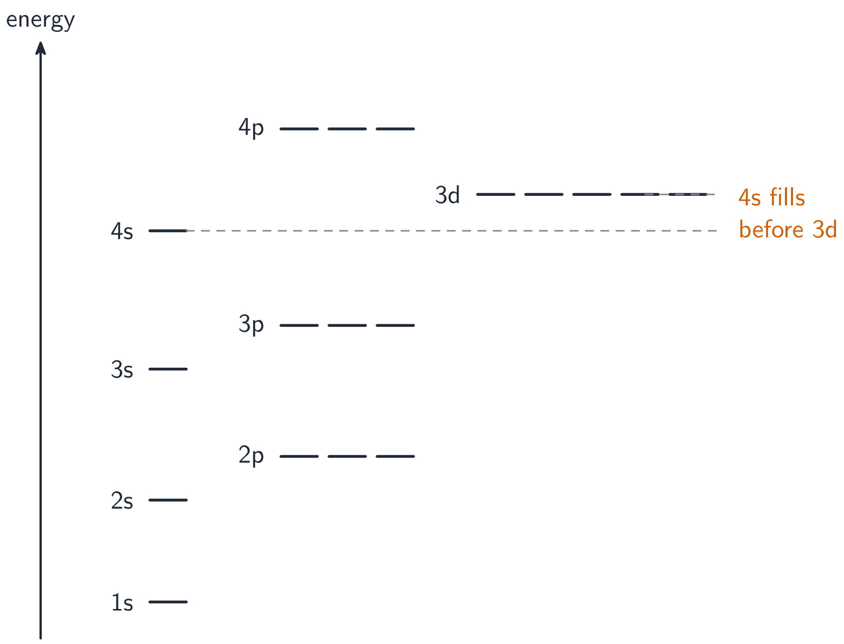
Build the skills to answer exam questions on **electrons, energy levels and atomic orbitals** — **shells, sub-shells and orbitals** 壳层、亚层和轨道, the order of filling, **electronic configurations** 电子排布, and orbital shapes.

You must be able to:

- describe the orbitals and electron capacity of s, p and d sub-shells
- write the electronic configuration of an atom or ion (full and shorthand)
- use the electrons-in-boxes notation and describe s and p orbital shapes

1 Worked examples

Sub-shells and filling order

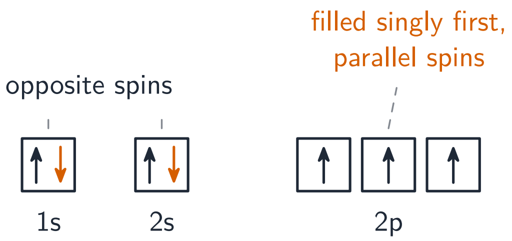


Order of rising energy: 1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p (4s fills before 3d)

sub-shell	orbitals	max electrons
s	1	2
p	3	6
d	5	10

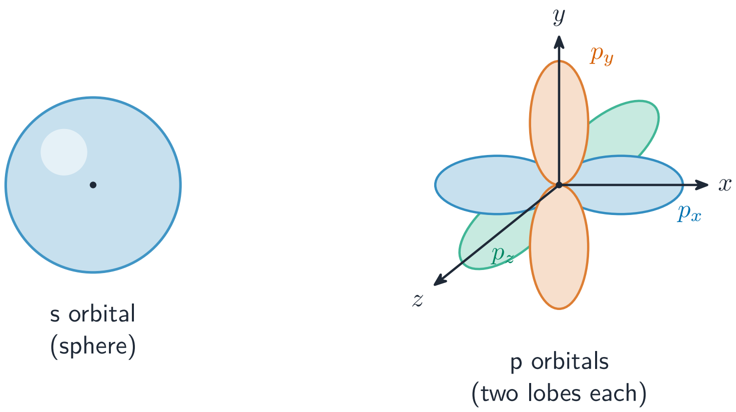
■ Electronic configuration

For iron (Fe, $Z = 26$): $1s^2\,2s^2\,2p^6\,3s^2\,3p^6\,3d^6\,4s^2$, or shorthand $[Ar]\,3d^6\,4s^2$. For a transition-metal ion, remove the **4s electrons first**: $Fe^{3+} = [Ar]\,3d^5$.



Paired electrons point opposite ways; within a sub-shell, orbitals fill singly first (parallel spins)

■ Orbital shapes



An s orbital is a sphere; each p orbital is a dumbbell along one axis

■ Sub-shells, orbitals, and the two rules that fix an order

An **orbital** 轨道 is a region that can hold **at most two electrons**, and only if they have **opposite spins**. The sub-shells and their capacities:

Sub-shell	Orbitals	Maximum electrons	Shape
s	1	2	spherical
p	3	6	dumb-bell, along x, y, z
d	5	10	more complex

The filling order follows increasing energy, and the one crossover that matters is that **4s fills before 3d**:

$$\text{1s 2s 2p 3s 3p } \mathbf{4}\text{s 3d 4p}$$

Hund's rule: within a sub-shell, electrons occupy the orbitals **singly with parallel spins** before any orbital is doubled up, because electrons repel. That is why an electrons-in-boxes diagram for nitrogen ($2p^3$) shows three separate up-arrows, not one pair and one single.

Two exceptions, both explained the same way — a half-filled or filled d sub-shell is more stable: **chromium** is $[Ar]\,3d^5 4s^1$ and **copper** $[Ar]\,3d^{10} 4s^1$.

△ **When an ion forms, the 4s electrons leave FIRST**, even though 4s filled first. Fe is $[Ar]\,3d^6 4s^2$ but Fe^{2+} is $[Ar]\,3d^6$ and Fe^{3+} is $[Ar]\,3d^5$.

Ionisation energy is the evidence. Successive ionisation energies rise steadily within a shell and **jump sharply** when the next electron must come from a shell closer to the nucleus. Counting the electrons removed before the big jump gives the **group** — a jump after the second electron means Group II.

Worked example. Write the electronic configuration of a Cu^{2+} ion, and explain the shape of the graph of successive ionisation energies for magnesium.

1. Cu is [Ar] $3d^{10}4s^1$ (an exception); remove the 4s electron first, then one 3d: Cu^{2+} is [Ar] $3d^9$.
2. Magnesium's first two ionisation energies are relatively low and close together (both 3s electrons). The third shows a large jump, because that electron comes from the 2p sub-shell — closer to the nucleus and less shielded — which is the evidence that magnesium is in Group II.

2 Practice

2.1 State the maximum number of electrons in (a) a p sub-shell and (b) a d sub-shell. [2]

2.2 Write the full electronic configuration of a calcium atom ($Z = 20$). [1]

2.3 State the maximum number of electrons in a p sub-shell and explain why. [2]

2.4 Give the electronic configuration of a Cr atom and explain why it is an exception. [2]

2.5 Explain what a large jump between successive ionisation energies tells you. [2]

3 Exam-style questions

3.1 Which sub-shell is filled **before** the 3d sub-shell? [1]

A	B
C	D

A 3p
B 4s
C 4p
D 4d

3.2 What is the shape of a p orbital? [1]

A	B
C	D

A spherical
B dumbbell (two lobes)
C a flat ring
D a cube

3.3 (a) Write the shorthand electronic configuration of an iron atom ($Z = 26$). [1]

(b) Write the electronic configuration of the Fe^{3+} ion, and explain which electrons are lost first. [2]

3.4 Using electrons-in-boxes, explain why the three 2p electrons of nitrogen occupy separate orbitals with parallel spins. [2]

3.5 (a) Give the full electronic configuration of a vanadium atom (proton number 23). [2]

(b) Give the electronic configuration of a V^{3+} ion, and state which electrons are lost first. [2]

(c) Draw an electrons-in-boxes diagram for the 3d and 4s sub-shells of a vanadium atom, and state the rule that determines the arrangement. [3]

(d) The first six ionisation energies of an element, in kJ mol^{-1}, are 786, 1580, 3230, 4360, 16 100, 19 800. Deduce the group of the element and explain your reasoning. [3]

(e) Explain why the first ionisation energy of aluminium is lower than that of magnesium, despite aluminium having a greater nuclear charge. [3]