

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

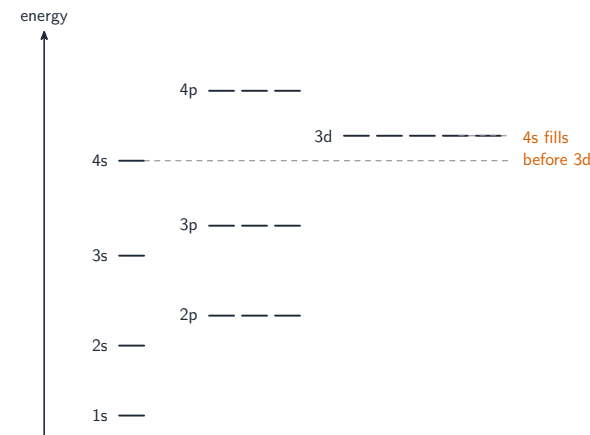
Build the skills to answer exam questions on **electrons, energy levels and atomic orbitals** — **shells, sub-shells and orbitals** 壳层、亚层和轨道, the order of filling, **electronic configurations** 电子排布, and orbital shapes.

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

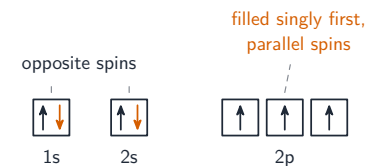


Order of rising energy: $1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p$ ($4s$ fills before $3d$)

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

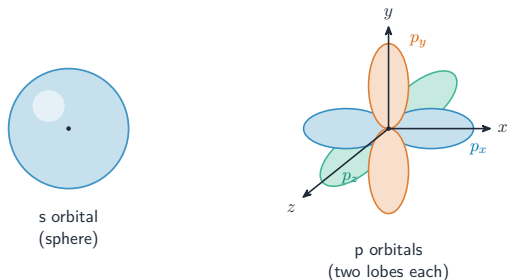
■ Electronic configuration

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



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**:

1s 2s 2p 3s 3p **4s** 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 $[\text{Ar}] 3d^5 4s^1$ and **copper** $[\text{Ar}] 3d^{10} 4s^1$.

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

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 $[\text{Ar}] 3d^{10} 4s^1$ (an exception); remove the 4s electron first, then one 3d: Cu^{2+} is $[\text{Ar}] 3d^9$.
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 3p
- B 4s
- C 4p
- D 4d

3.2 What is the shape of a p orbital?

[1]

- 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]

Solutions

2.1 (a) 6; (b) 10.

2.2 $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$.

2.3 Six; a p sub-shell has three orbitals and each orbital holds at most two electrons, with opposite spins.

2.4 $[\text{Ar}] 3d^5 4s^1$; a half-filled d sub-shell is more stable than the expected $3d^4 4s^2$.

2.5 The next electron is being removed from a shell closer to the nucleus, which is less shielded and more strongly attracted, so far more energy is needed.

3.1 B. 4s is slightly lower in energy than 3d, so it fills first.

3.2 B. A p orbital is a dumbbell (two lobes).

3.3 (a) $[\text{Ar}] 3d^6 4s^2$.

(b) $[\text{Ar}] 3d^5$; the 4s electrons are removed before the 3d electrons.

3.4 each electron is negative and they repel; occupying separate orbitals keeps them apart, lowering repulsion — the lowest-energy (most stable) arrangement.

3.5 (a) $1s^2 2s^2 2p^6 3s^2 3p^6 3d^3 4s^2$.

(b) $[\text{Ar}] 3d^2$; the two 4s electrons are lost first, then one 3d electron.

(c) 4s shown as one box with two opposed arrows; 3d shown as five boxes with three single arrows all pointing the same way; Hund's rule — electrons occupy orbitals singly with parallel spins before pairing, because they repel.

(d) Group IV; the large jump comes between the fourth and fifth ionisation energies, so four electrons are removed from the outer shell before the next must come from a shell closer to the nucleus.

(e) Magnesium's outer electron is in a 3s orbital and aluminium's in a 3p orbital; the 3p sub-shell is slightly higher in energy and better shielded by the 3s electrons; that outweighs the extra proton, so less energy is needed to remove it.