

Electronic Structure

Quantum mechanics provides a far more complete picture of how electrons are arranged in atoms. Solutions to the *Schrödinger equation* describe the probability of finding an electron in a given volume of space. These individual volumes of space are known as **atomic orbitals**.

Definition (Atomic Orbital) — A volume of space with a maximum of two electrons of opposite spin, where there is at least a 90% probability of finding an electron.

Electron arrangement can be summarised by three basic principles:

1. **Aufbau's Principle:** energy levels are not entered until those below them are filled.
2. **Pauli's Exclusion Principle:** orbitals can hold a maximum of two electrons, provided they have opposite spin.
3. **Hund's Rule:** orbitals of the same energy remain singly occupied before pairing up.

There are different types of orbitals: **s**-, **p**-, **d**- and **f**- orbitals. Each type of orbital has a different shape.

- **s-orbital:** the electron cloud is within a spherical shape. Each shell contains one s-orbital.
- **p-orbital:** the electron cloud is within a 'dumb-bell' shape. There are three p-orbitals in a shell orthogonal to each other - p_x , p_y and p_z .
- **d-orbital** and **f-orbital:** these form much more complex shapes with five d-orbitals and seven f-orbitals in a shell.

Electronic structure can be broken down into shells, also known as energy levels, and **subshells**. Within a shell, orbitals of the same type are grouped together as subshells.

Shell	Subshells	# of e ⁻ s in subshells	# of e ⁻ s in shell
1	1s	2	2
2	2s + 2p	2 + 6	8
3	3s + 3p + 3d	2 + 6 + 10	18
4	4s + 4p + 4d + 4f	2 + 6 + 10 + 14	32

In general, the number of electrons in the n th shell is $2n^2$. Below are the electron configurations for the first 30 elements. The '[Ar]' notation is used for speed and it simply means input the electron configuration of argon (or the other respective noble gas) there.

1	H	1s ¹	16	S	[Ne] 3s ² 3p ⁴
2	He	1s ²	17	Cl	[Ne] 3s ² 3p ⁵
3	Li	[He] 2s ¹	18	Ar	[Ne] 3s ² 3p ⁶
4	Be	[He] 2s ²	19	K	[Ar] 4s
5	B	[He] 2s ² 2p ¹	20	Ca	[Ar] 4s ²
6	C	[He] 2s ² 2p ²	21	Sc	[Ar] 3d ¹ 4s ²
7	N	[He] 2s ² 2p ³	22	Ti	[Ar] 3d ² 4s ²
8	O	[He] 2s ² 2p ⁴	23	V	[Ar] 3d ³ 4s ²
9	F	[He] 2s ² 2p ⁵	24	Cr	[Ar] 3d ⁵ 4s ¹
10	Ne	[He] 2s ² 2p ⁶	25	Mn	[Ar] 3d ⁵ 4s ²
11	Na	[Ne] 3s ¹	26	Fe	[Ar] 3d ⁶ 4s ²
12	Mg	[Ne] 3s ²	27	Co	[Ar] 3d ⁷ 4s ²
13	Al	[Ne] 3s ² 3p ¹	28	Ni	[Ar] 3d ⁸ 4s ²
14	Si	[Ne] 3s ² 3p ²	29	Cu	[Ar] 3d ¹⁰ 4s ¹
15	P	[Ne] 3s ² 3p ³	30	Zn	[Ar] 3d ¹⁰ 4s ²

Note that when filling up, 4s electrons are occupied before 3d electrons, and similarly 5s fill up before 4d. This is because the 4s and 5s are lower in energy than the 3d and 4d respectively.

However, in forming cations, electrons in the 4s orbital are lost before electrons in the 3d orbital *etc.* Hence, the electronic configuration of say Ti^{2+} would be $[\text{Ar}] 3d^2$, not $[\text{Ar}] 4s^2$.

As with much in chemistry, there are always exceptions to the rule. In this case, **copper** and **chromium**. They do not have the expected electron structure, but it's one of those things that you've got to learn.