



Chemistry and the material world

123.102

Lecture 1

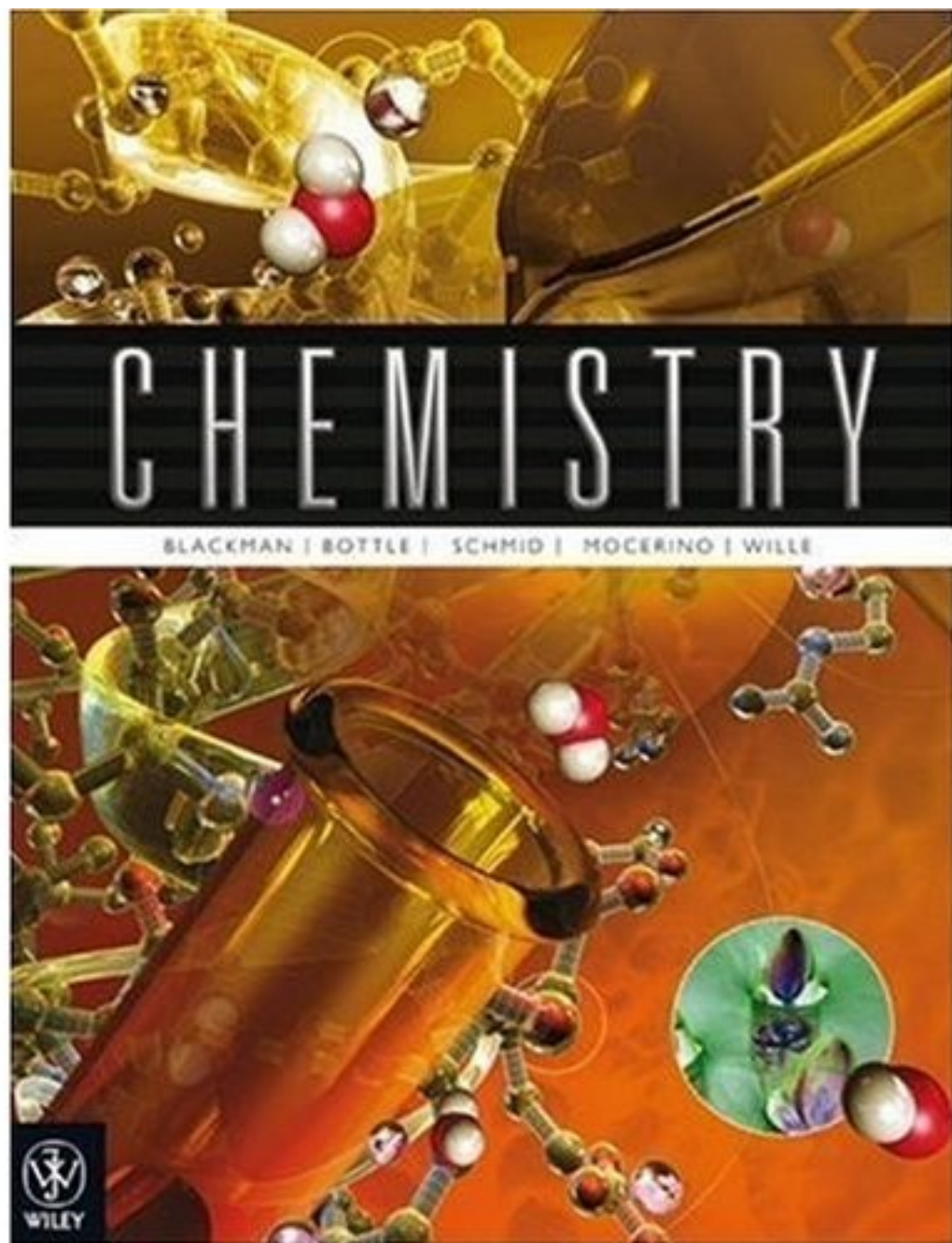


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 - ◆ <http://ctcp.massey.ac.nz/>
- ◆ Fire safety
- ◆ Class representatives
 - ◆ Looks good on your CV
 - ◆ You will receive training by ASA (Wed, 6th August)
 - ◆ There will be a certificate and a class rep party at the end of the year



- ◆ Stick to the study guide:
 - ◆ Everything you need to know in order to pass is in there!
 - ◆ All the rules and requirements are in there too.
 - ◆ Use other resources if you don't understand or want to know more, but always use the study guide as a starting point – don't get lost in detail.
- ◆ Use the online resources on WebCT:
 - ◆ There are additional tutorials and an online version of the study guide.
 - ◆ There are old exam questions and answers!
 - ◆ Use the additional tutorials online.
 - ◆ Ask questions in the online forum.



Chemistry

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- ◆ Introduction
 - chemistry
 - atomic theories
 - electrons
- ◆ description of electrons
 - orbitals
 - atomic orbitals
 - molecular orbitals
- ◆ electron configurations
 - atomic energy level diagrams
 - configurations for atoms and ions
 - valence electrons



“Chemistry is the science concerned with the composition, structure and properties of matter, as well as the changes it undergoes during reactions.”

en.wikipedia.org

“Chemistry is the science of all substances and their transformations”

University Federico II of Naples, Italy

“Chemistry is the science of matter and its interactions with energy”

awesomelibrary.org

Qualitative approach

Description in terms of words
Understanding through analogy
and conceptual models

Quantitative approach

Description in terms of numbers
Understanding through
mathematics



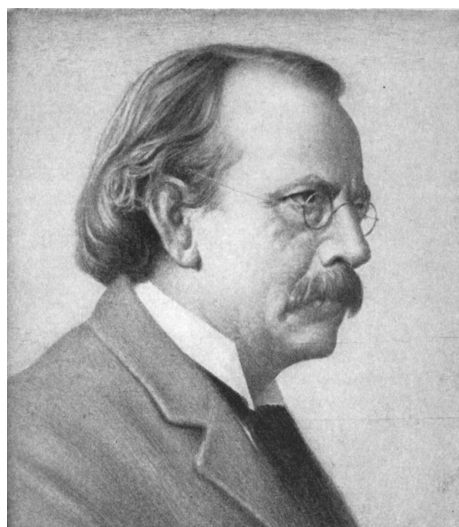
Democritus 5th century BC, Greece

- ἄτομος from “a-” un- or not- “-tomos” cuttable.
- They are immutable (they do not change).
- They are indivisible (they cannot be broken into smaller parts).
- They can have different sizes and shapes(!).
- They are all made of the same material.

- ◆ They are immutable (they do not change).
- ◆ They are indestructible (they cannot be destroyed).
- ◆ Atoms are the same for each chemical element (weight).
- ◆ They can combine to form chemical compounds (molecules).

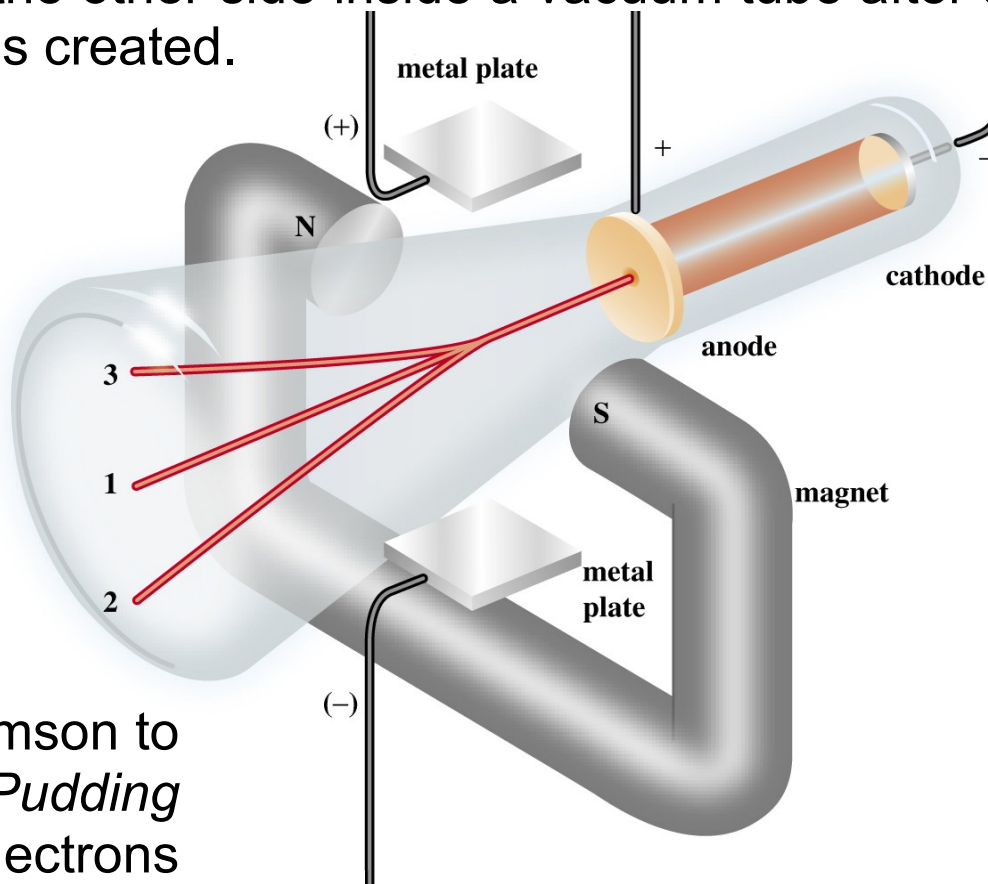
John Dalton
1766 – 1844, England





J. J. Thomson
1856 – 1940,
England

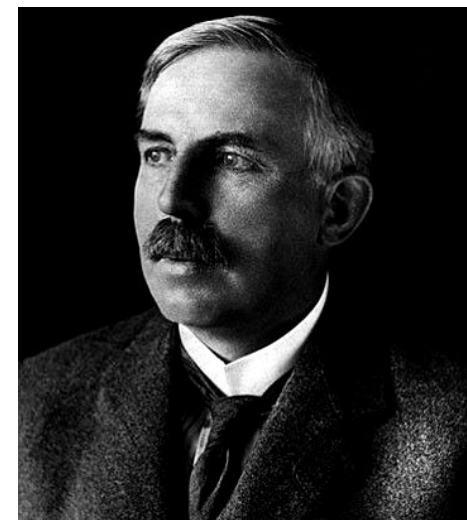
Thomson investigated cathode ray tubes. Where *cathode rays* are emitted from a heated cathode and beam to an anode on the other side inside a vacuum tube after an electrical potential is created.



By measuring the deflection in an electrical field he could show that the beam consisted of negatively charged particles — electrons.

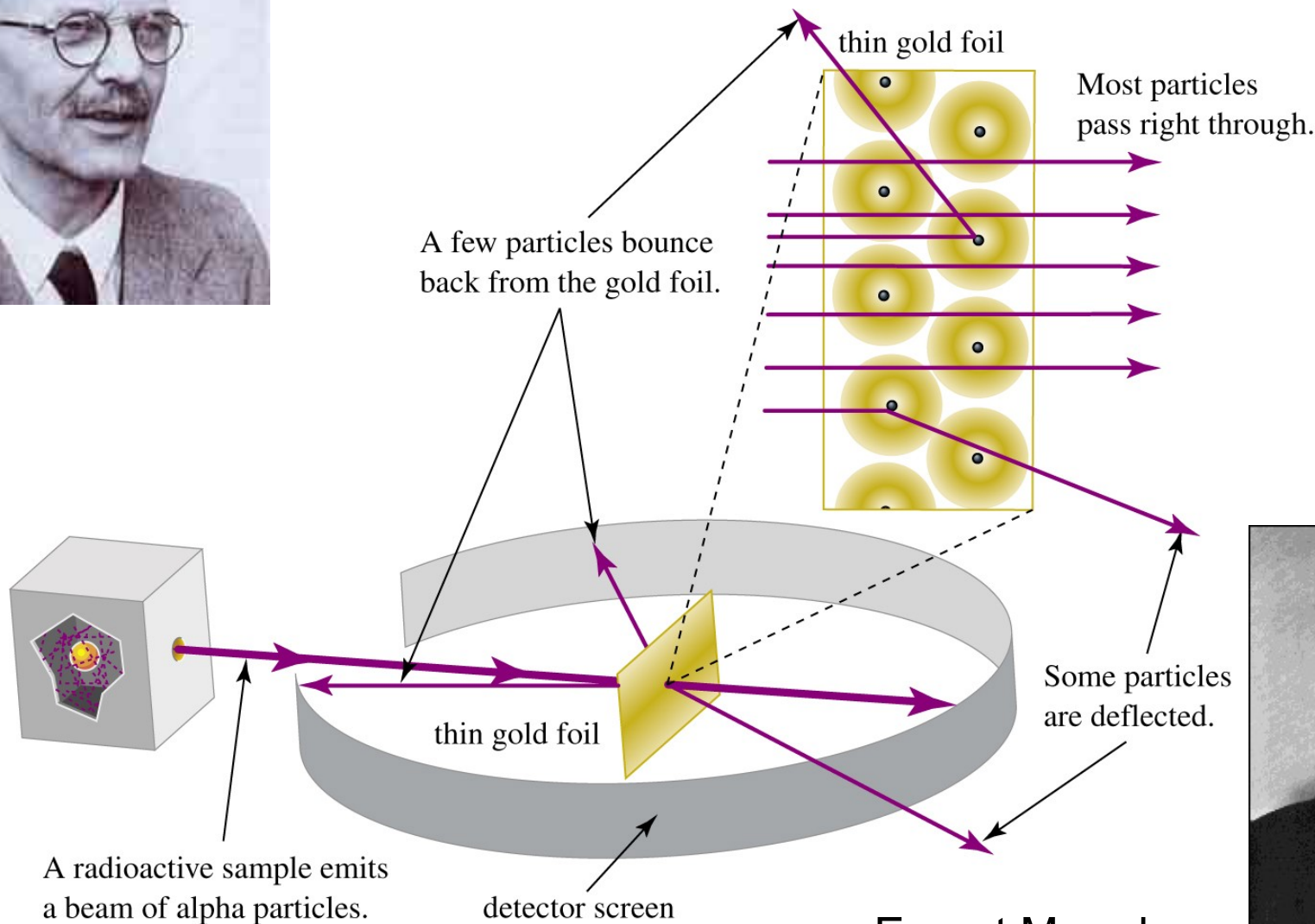
The results lead Thomson to the so called *Plum Pudding model* where the electrons in atoms would be neutralized by a positive charge cloud in which electrons could rotate freely.

Ernest Rutherford
1871 – 1937, New Zealand

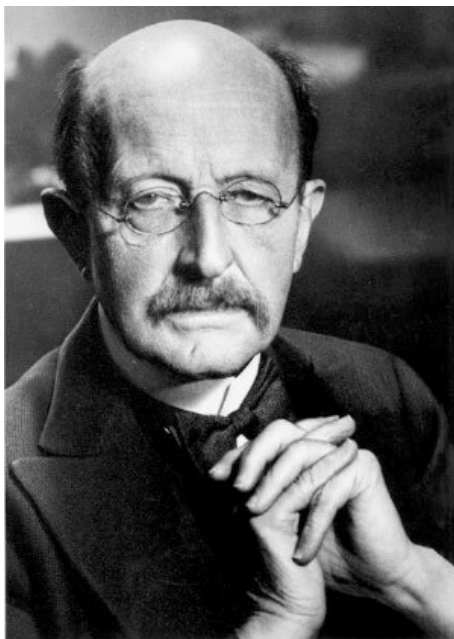




Hans Geiger
1882 – 1945, Germany



Ernest Marsden
1889 – 1970, New Zealand

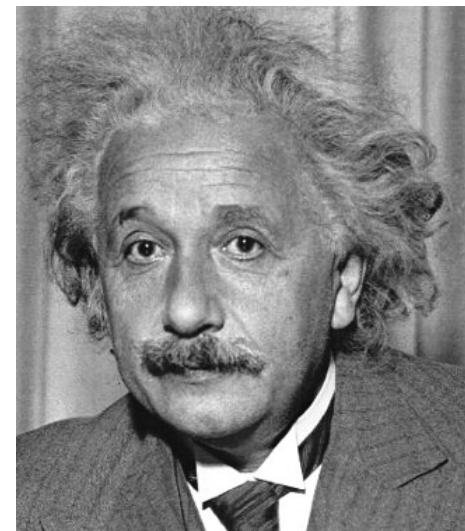


Max Planck
1858 – 1947, Germany

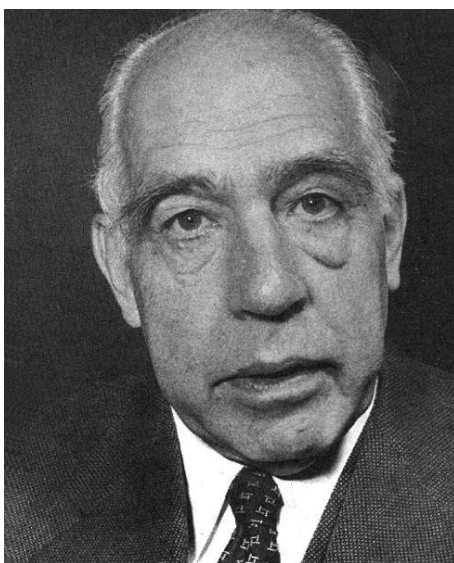
In 1900 Planck formulates his
quantum hypothesis

$$E = h\nu = \hbar\omega$$

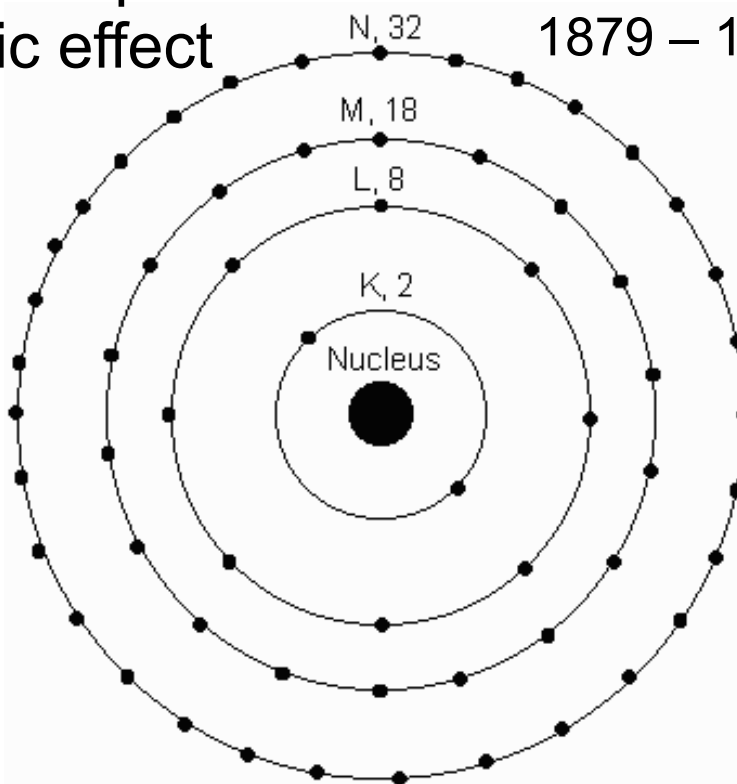
In 1905 Einstein explains
the photoelectric effect



Albert Einstein
1879 – 1955, Germany



Niels Bohr
1885 – 1962,
Denmark



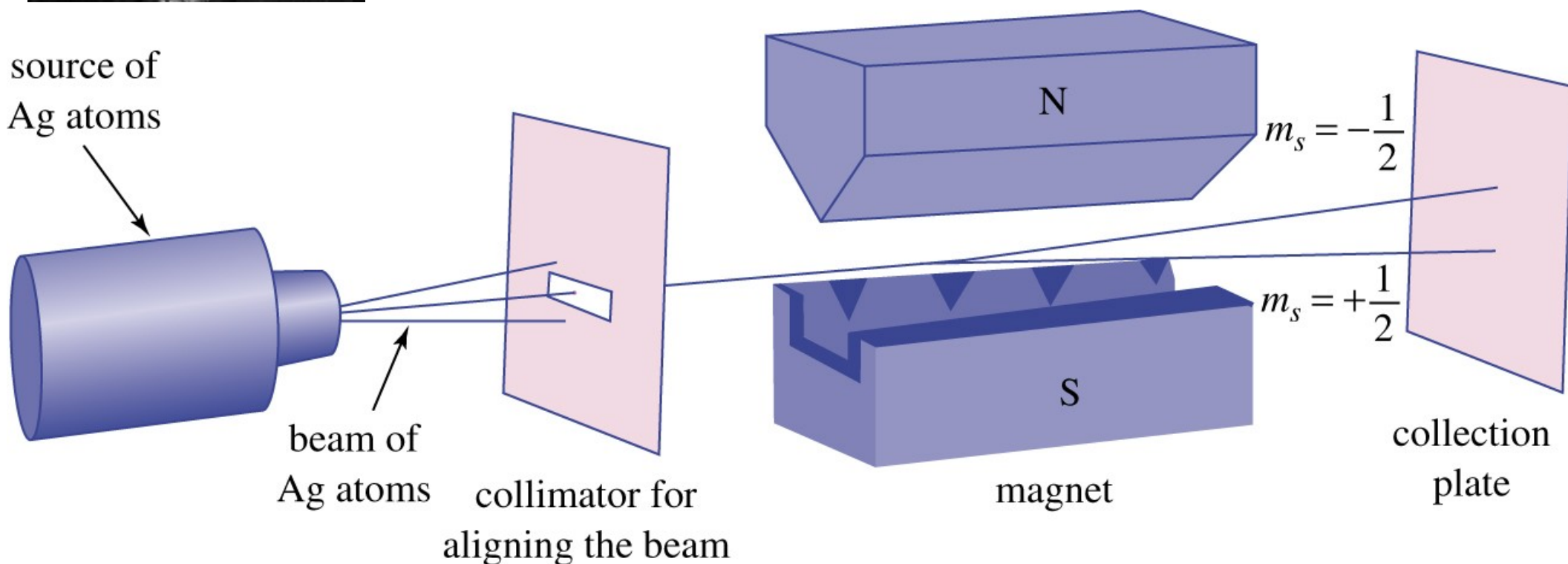
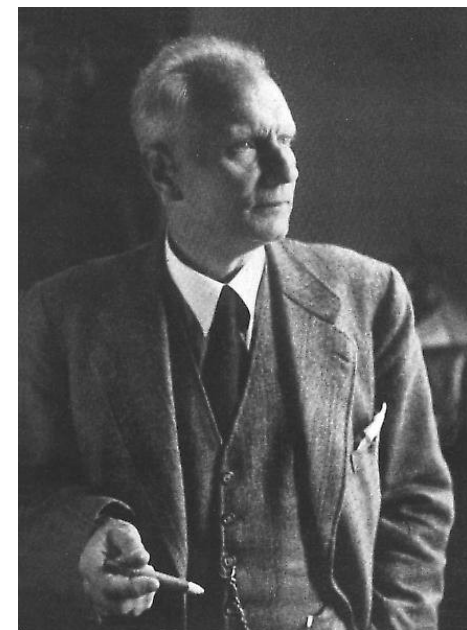


Otto Stern
1888 – 1969, Germany

Electrons have either:

- ◆ spin up (\uparrow) or down (\downarrow)
- ◆ alpha (α) spin or beta (β) spin

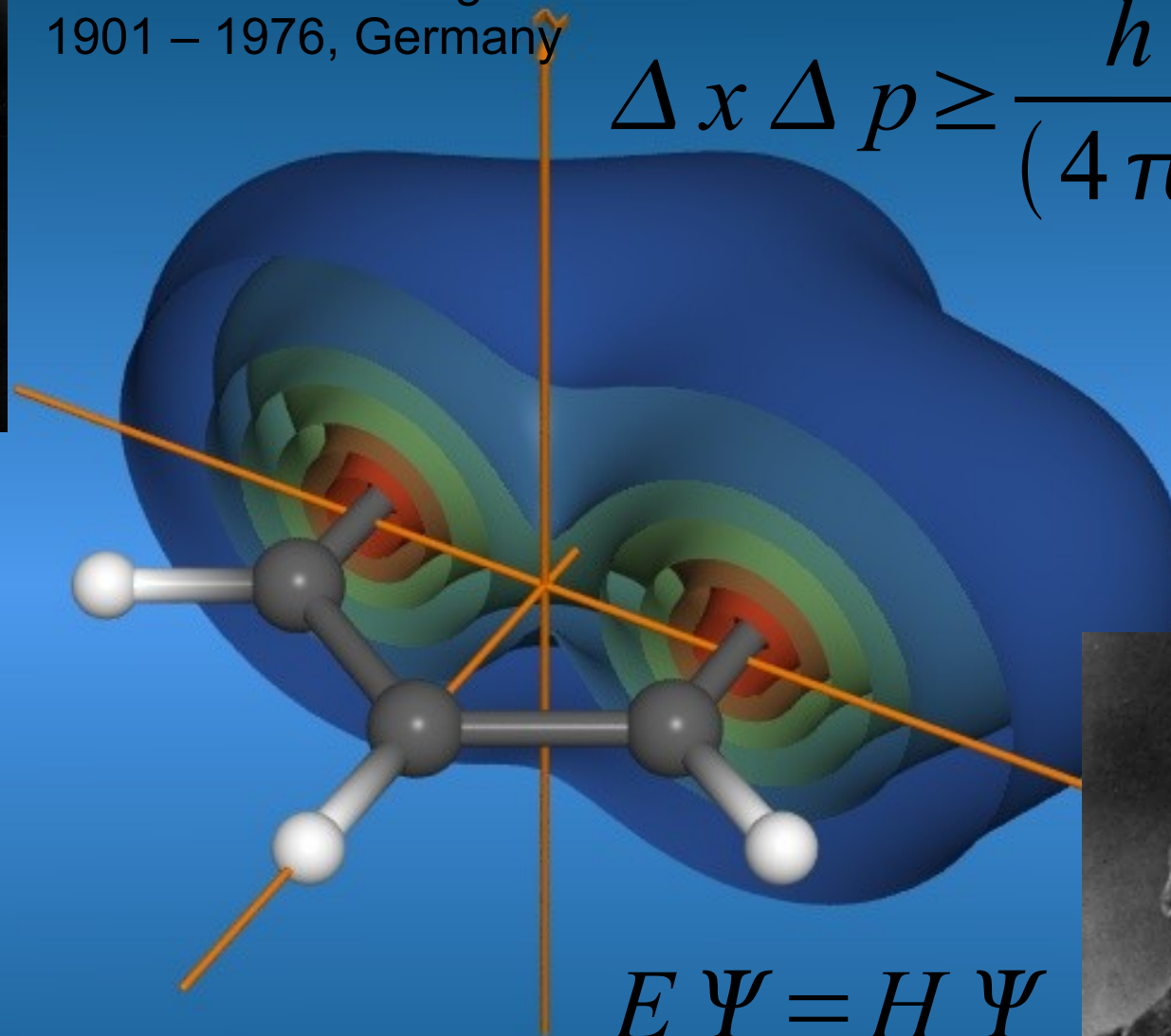
Walter Gerlach
1889 – 1979, Germany





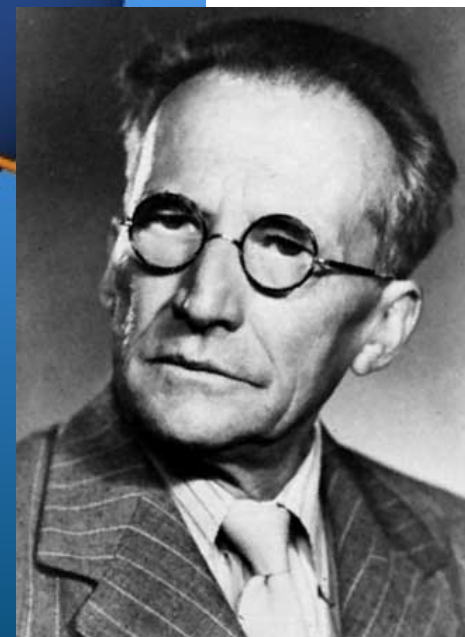
Werner Heisenberg
1901 – 1976, Germany

$$\Delta x \Delta p \geq \frac{h}{(4\pi)}$$



$$E \Psi = H \Psi$$

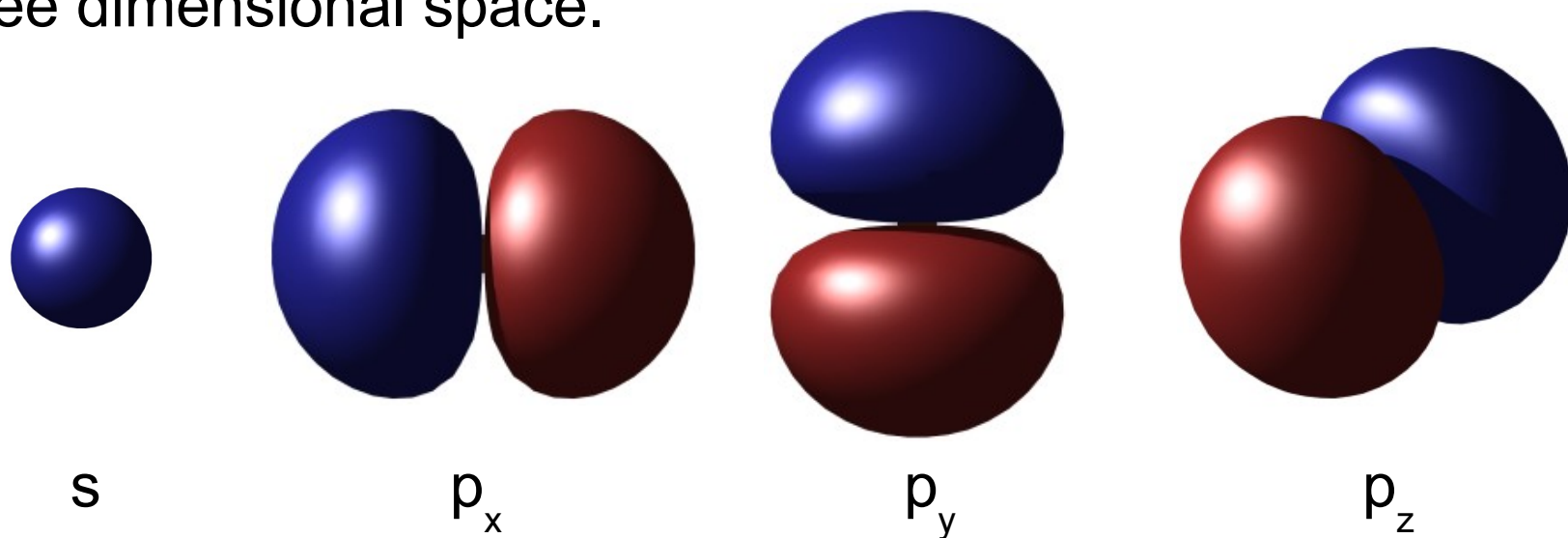
Erwin Schrödinger
1887 – 1961, Germany





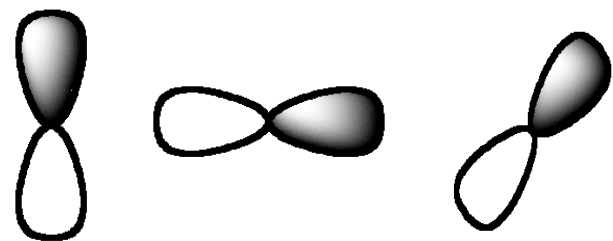
- ◆ Democritus
 - ◆ Atoms are unchangeable and cannot be broken into smaller parts.
 - ◆ Atoms are all made of the same material.
- ◆ Dalton
 - ◆ Atoms are unchangeable and cannot be broken into smaller parts.
 - ◆ Only atoms of the same element are made of the same material.
 - ◆ Compounds can be formed by combining atoms.
- ◆ Bohr
 - ◆ All Atoms are made of a very small nucleus made of protons and neutrons and electrons circling around this nucleus in shells.
 - ◆ The number of protons in a nucleus determines which element the atoms belongs to.
- ◆ “*modern*”
 - ◆ Atomic nuclei are made of protons and neutrons which can undergo nuclear reactions.
 - ◆ Electrons are best described by a wave function. The total wave function of a system is made up of individual wave functions or *orbitals*.

Instead of two dimensional circular or elliptical orbits (like planets around the sun) electrons are best described by a wave-function which gives the probability of finding an electron at a given point in three dimensional space.



A plot of such a function which outlines the region of space which an electron occupies for about 90% of the time are called *orbital plots* or often just *orbital*.

Atomic orbitals of hydrogen



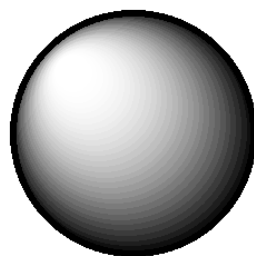
3p

Energy

-0.056

Radius

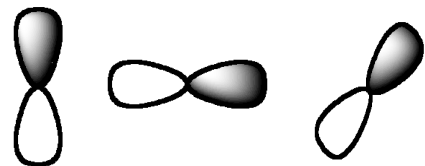
12.0



3s

-0.056

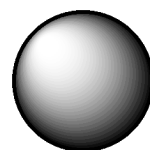
13.1



2p

-0.125

4.0



2s

-0.125

5.2



1s

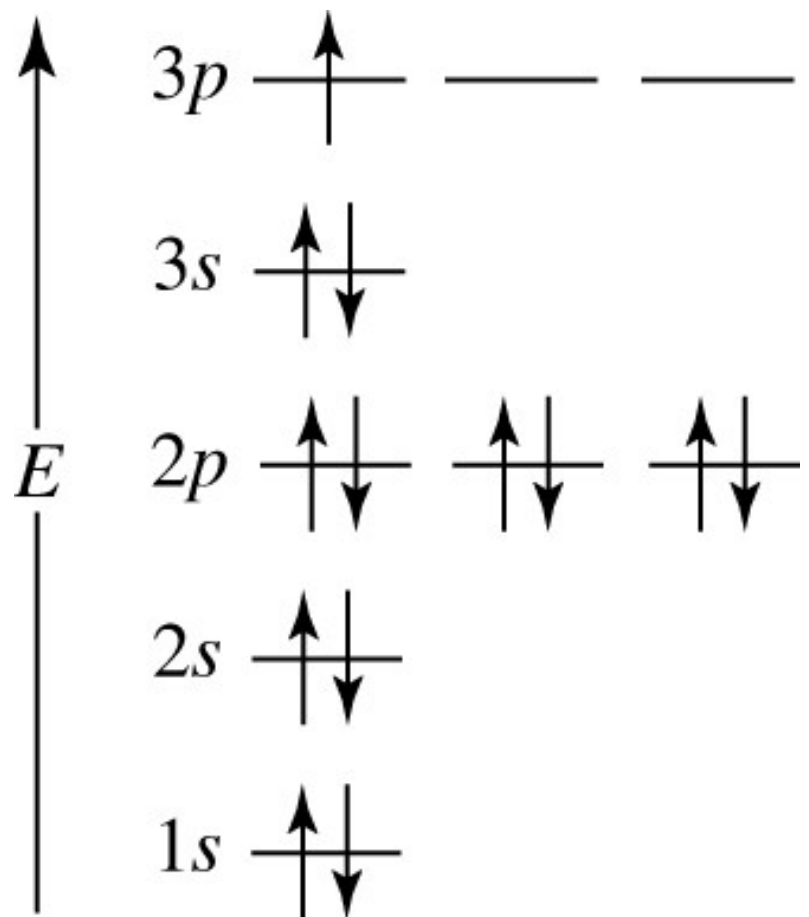
-0.500

1.0

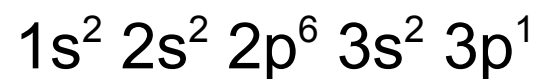
Atom	1s	2s	2p	3s	3p
H	-0.50				
He	-0.92				
Li	-2.49	-0.20			
Be	-4.73	-0.31			
B	-7.70	-0.54	-0.31		
C	-11.35	-0.83	-0.43		
N	-15.67	-1.16	-0.57		
O	-20.71	-1.42	-0.71		
F	-26.41	-1.67	-0.84		
Ne	-32.78	-1.93	-0.85		
Na	-40.49	-2.79	-1.52	-0.18	
Mg	-49.04	-3.77	-2.28	-0.25	
Al	-58.50	-4.91	-3.23	-0.42	-0.21
Si	-68.82	-6.16	-4.27	-0.62	-0.30
P	-79.98	-7.52	-5.42	-0.84	-0.39
S	-92.01	-9.01	-6.71	-0.99	-0.48
Cl	-104.89	-10.61	-8.10	-1.14	-0.57
Ar	-118.61	-12.32	-9.57	-1.28	-0.59

- ◆ Orbitals in the same shell (3s vs. 3p) are not degenerate anymore.
- ◆ The higher the nuclear charge (the larger the number of protons Z), the more the electrons are attracted towards it. Thus any given orbital shrinks with growing Z and the corresponding energy becomes more negative.
- ◆ The orbitals can be ordered according to their energy:

$$1s < 2s < 2p < 3s < 3p$$



Atomic energy level diagram

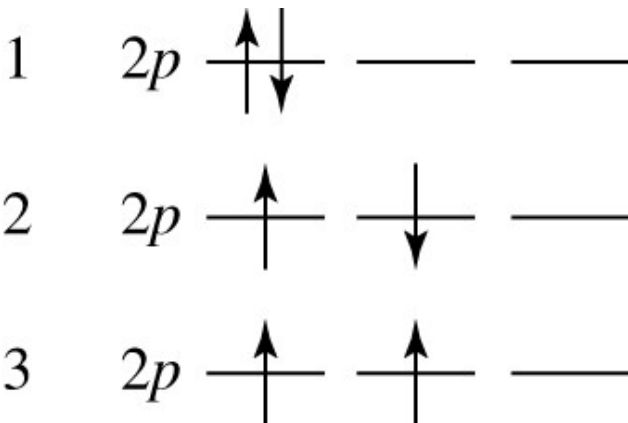


Atomic electron configuration



In order to arrive at the ground state, the lowest energy state, it is necessary to follow some simple rules:

- ◆ Electrons occupy the lowest energy level first (also called the *Aufbau Principle*)
- ◆ No more than one alpha (or spin up) and one beta (or spin down) electron can occupy a particular orbital at any time (also called *Pauli Exclusion Principle*)
- ◆ If degenerate orbitals are available, they will be singly occupied first, then doubly.





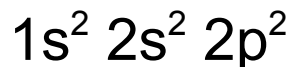
Example 1 = neutral atoms

The electron configuration of carbon (C), $Z = 6$ is as follows:

- ◆ The nuclear charge $Z = 6$ means that there are 6 electrons to distribute
- ◆ They are filled, one after another into the Atomic Energy Level Diagram

$$1s < 2s < 2p < 3s < 3p$$

We get:





Example 2 – cations

Cations are positively charged. They have at least one electron less than their nuclear charge.

The electron configuration of Li^+ , $Z = 3$ is as follows:

- ◆ The nuclear charge $Z = 3$ means that neutral lithium has 3 electrons to distribute.
- ◆ Since we are dealing with an atom which has one positive charge. There is one electron less to consider.

Those two electron are filled, one after another into the Atomic Energy Level Diagram

$$1s < 2s < 2p < 3s < 3p$$

We get:





Example 3 – anions

Anions are negatively charged. They have at least one electron more than their nuclear charge.

The electron configuration of F^- , $Z = 9$ is as follows:

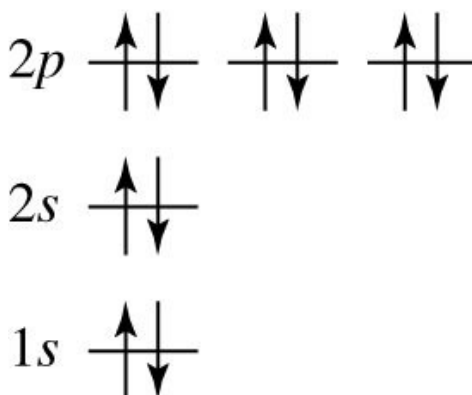
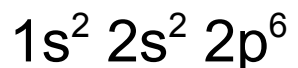
- ◆ The nuclear charge $Z = 9$ means that neutral fluorine has 9 electrons to distribute.
- ◆ Since we are dealing with an atom which has one negative charge. There is one electron more to consider.

Those ten electron are filled, one after another into the Atomic Energy Level

Diagram

$$1s < 2s < 2p < 3s < 3p$$

We get:





Chemical reactions usually only involve the outermost electrons these electrons are called *valence electrons*.

These electrons reside in the *valence shell*.

The valence shell is the highest-energy shell that (in the ground state) contains electrons.

Example:

F: $1s^2 2s^2 2p^5$	the highest energy shell is shell 2
C: $1s^2 2s^2 2p^2$	the highest energy shell is shell 2
H: $1s^1$	the highest energy shell is shell 1

The *valence configuration* is the electron configuration of the valence shell.

Example:

H: $1s^1$	the valence configuration is s^1 .
Li: $1s^2 2s^1$	the valence configuration is s^1 .
Na: $1s^2 2s^2 2p^6 3s^1$	the valence configuration is s^1 .



Today we covered:

- ◆ The properties of electrons
 - ◆ They are negatively charged.
 - ◆ They have a spin (either up or down).
- ◆ The shapes of s and p orbitals
 - ◆ s orbitals are spherically symmetric (“round”).
 - ◆ p orbitals have two lobes with opposite sign along the axes.
 - ◆ p orbitals are also triply degenerate.
- ◆ Atomic energy levels and electron configurations (first 18 elements)
 - ◆ $1s < 2s < 2p < 3s < 3p$
 - ◆ Electrons are filled into orbitals according to rules (Aufbau Principle, Pauli Exclusion Principle, Hund's Rule).
- ◆ Valence electrons
 - ◆ Valence electrons are the outermost electrons of an atom.
 - ◆ The valence shell is the highest energy shell that contains electrons.