Chem 103, Section F0F
Unit II - Quantum Theory and Atomic Structure
Lecture 8

- More on the periodic table
- Some characteristics of atoms that have more than 1 electron
- The quantum mechanical model of the atom and the periodic table

Lecture 8 - Electron Configuratioin

- Reading in Silberberg
  - Chapter 8, Section 1 *Development of the periodic table*
  - Chapter 8, Section 2 *Characteristics of many-electron atoms*
  - Chapter 8, Section 3 The quantum-mechanical model and the periodic table

Lecture 8 - Introduction

The periodic law gave rise to the periodic table

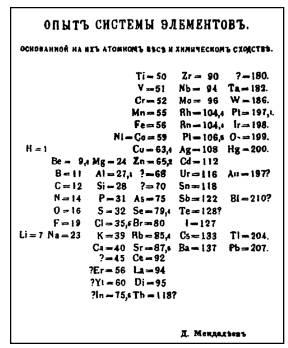
- In the mid to late 1800's scientists, such as Demtri Mendeleev, where looking for ways to organize their knowledge of the the properties of the known elements.
  - This led to the creation of the Periodic Table.
- In this lecture we will see that the discoveries of the early 1900's, which led to the quantum mechanical model for the structure of the atom allows us to see how the arrangement of the elements in the periodic table are intimately related to their **electronic configurations**.

Lecture 4 - The Atomic Theory Today

In the 19th century, investigators looked for ways to organize what was known about the various elements.

Dmitri Mendeleev (1836-1907) created one of the most useful arrangements, in which the elements were arranged by mass.

- In this arrangement, Mendeleev also grouped elements with similar physical and chemical properties.



Lecture 8 - Periodic Law

One of the powerful aspect of Mendeleev's periodic table was it ability to predict the physical and chemical properties of elements yet to be discovered.

- For example:
  - Mendeleev was able to predict the properties of an element that he called "eka-silicon"
  - Later, when eka-silicon was isolated, it was found to have properties remarkably similar to those predicted by Mendeleev
    - This element is now called Germanium (Ge).

Lecture 8 - Periodic Law

The properties predicted for "eka-Silicon"

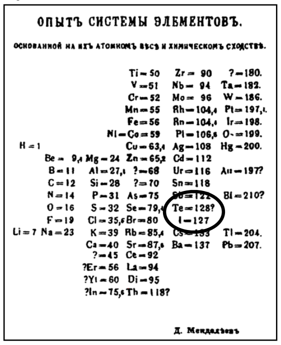
Table 8.1 Mendeleev's Predicted Properties of Germanium ("eka Silicon") and Its Actual Properties

Property	Predicted Properties of eka Silicon (E)	Actual Properties of Germanium (Ge)
Atomic mass	72 amu	72.61 amu
Appearance	Gray metal	Gray metal
Density	5.5 g/cm^3	5.32 g/cm^3
Molar volume	13 cm^3/mol	13.65 cm^3/mol
Specific heat capacity	0.31 J/g·K	0.32 J/g·K
Oxide formula	EO_2	GeO_2
Oxide density	4.7 g/cm^3	4.23 g/cm^3
Sulfide formula and solubility	ES_2; insoluble in H_2O; soluble in aqueous $(NH_4)_2S$	GeS_2; insoluble in H_2O; soluble in aqueous $(NH_4)_2S$
Chloride formula (boiling point)	ECl_4 (<100°C)	$GeCl_4$ (84°C)
Chloride density	1.9 g/cm^3	1.844 g/cm^3
Element preparation	Reduction of K_2EF_6 with sodium	Reduction of K_2GeF_6 with sodium

Lecture 8 - Periodic Law

Mendeleev's table was arranged by the atomic mass of the elements.

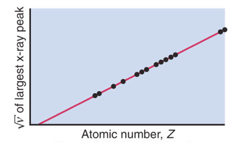
- There are some examples in Mendeleev's table where the elements are out of order according to their masses.
  - This is because Mendeleev recognized that properties should trump masses in determining the arrangement of the elements in the periodic table.
- Meendeleev's placement of Telurium (Te), with a mass of 128, ahead of Iodine (I), with a mass of 127, is one example.



Lecture 8 - Periodic Law

Henry Moseley (1887-1915)

- In the early 1900's, Henry Moseley discovered a way of determining the number of protons in an element by analyzing the X-rays emitted by an atom upon being bombarded by a beam of electrons.
- This allowed the periodic chart to now be arranged by atomic number, which displays no issues with ordering.



Lecture 8 - Many-Electron Atoms

Schrödinger's quantum-mechanical model allows for the electronic configurations of atoms containing more than one electron to be approximated.

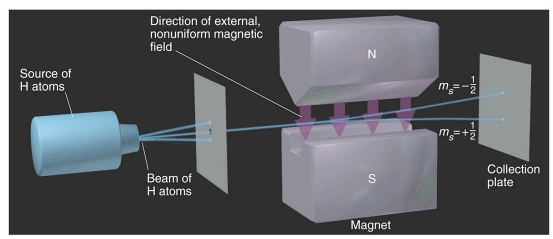
The addition of more than 1 electron requires three considerations to be made:

- The need for a forth quantum number, m_s.
- A limit on the number of electrons that can occupy a single orbital (**the exclusion rule**).
- The existence of a more complex set of energy levels.

Lecture 8 - Many-Electron Atoms

When a beam of hydrogen atoms passes through a strong magnetic field it splits into two beams.

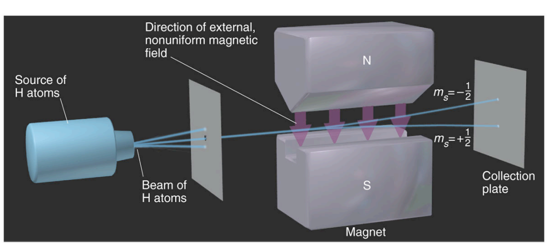
- This is due the 1 electron in hydrogen atoms having one of two possible "spins".



Lecture 8 - Many-Electron Atoms

Identifying electrons in many-electron atoms requires four quantum numbers

- *n*, *l*, m_l
- Plus a forth, m_s, **electron spin**, which is a property of the the electron.



Lecture 8 - Many-Electron Atoms

Identifying electrons in many-electron atoms requires four quantum number

- *n*, *l*, m_l
- Plus a forth, m_s, electron spin, which is a property of the the electron

Table 8.2 Summary of Quantum Numbers of Electrons in Atoms

Name	Symbol	Permitted Values	Property
Principal	n	Positive integers (1, 2, 3, …)	Orbital energy (size)
Angular momentum	l	Integers from 0 to $n - 1$	Orbital shape (The l values 0, 1, 2, and 3 correspond to *s*, *p*, *d*, and *f* orbitals, respectively.)
Magnetic	m_l	Integers from $-l$ to 0 to $+l$	Orbital orientation
Spin	m_s	$+\frac{1}{2}$ or $-\frac{1}{2}$	Direction of e^- spin

Lecture 8 - Many-Electron Atoms

Pauli exclusion principle: *No two electrons in the same atom can have the same four quantum numbers*.

- Named for Wolfgang Pauli, who was awarded the 1945 Nobel Prize in physics for his contribution to our understanding of the structure of the atom.
- This limits each orbital in an atom to containing only 2 electrons.
  - The two electrons must have opposite spins.

Wolfgang Pauli
(1900-1958)

Lecture 8 - Many-Electron Atoms

Energy level splitting.

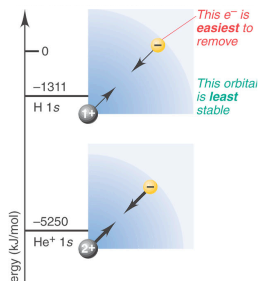
- Electrostatic interactions between electrons in atoms with more than one electron causes the energy levels to split into **sublevels**.

- The electrostatic effects include:
  - The effect of nuclear charge (*Z*)
  - The effect of electron repulsions and shielding on orbital energy
  - The effect of orbital shape on orbital energy (**penetration**)

Lecture 8 - Many-Electron Atoms

The effect of nuclear charge (Z)

- Higher nuclear charge lowers the energy of an energy level.

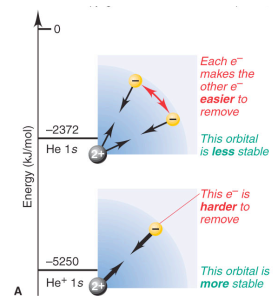


Comparing the *1s* orbital of H and He^+

Lecture 8 - Many-Electron Atoms

The effect of electron repulsions and shielding on orbital energy

- The electrons feel not only the attraction of the nucleus, but also the repulsion of the other electrons.

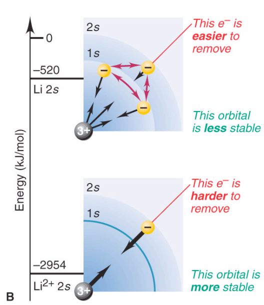


Electron repulsion

Lecture 8 - Many-Electron Atoms

The effect of electron repulsions and shielding on orbital energy

- The electrons feel not only the attraction of the nucleus, but also the repulsion of the other electrons.
- Shielding by inner elecrons greatly lowers the effective nuclear charge (Z_{eff}).

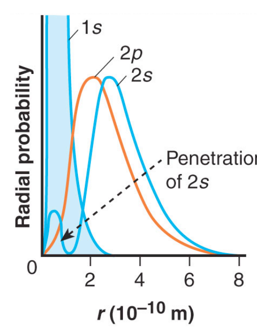


Electron shielding

Lecture 8 - Many-Electron Atoms

The effect of orbital shape on orbital energy (**penetration**)

- The different orbitals, which are defined by the *l* quantum number, place the electrons at different distances from the nucleus,
  - The more stable orbitals are the ones that come closer to the nucleus.
- Sublevel energies:
  - $s < p < d < f$

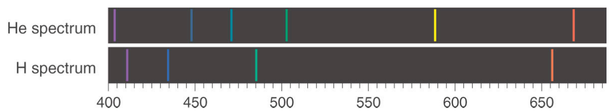


Orbital penetration

Lecture 8 - Many-Electron Atoms

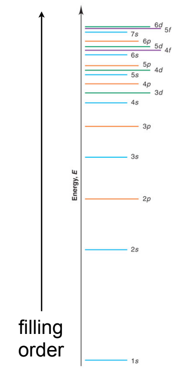
Multiple electrons in the same atoms leads to
- electron-electron repulsion
- nuclear shielding
- energy-level splitting

These effects lead to more energy levels that predicted by the Bohr model
- These additional energy levels are observed in the atomic spectra of atoms with more than one electron.



Lecture 8 - Many-Electron Atoms

Energy-level splitting defines the order in which the electrons are filled



Lecture 8 - Quantum Mechanical Model of the Periodic Table

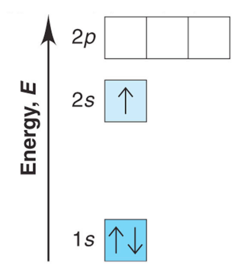
The electron configuration for an atom is a list of the orbitals that each of the electrons in the atom occupies.
- We will focus on the **ground state** configuration, which places all of the electrons in the orbitals with the lowest possible energies.

This list is most easily constructed by
- starting with a naked nucleus with the desired atomic number, *Z*
- then adding *Z* electrons, one at a time
  - placing each in the available orbital having the lowest energy.

This approach is called the **aufbau principle** ("to build up")

Lecture 8 - Quantum Mechanical Model of the Periodic Table

This can be done using orbital diagrams
- Here is the orbital diagram for Lithium (*Z* = 3)



The shorthand convention for representing the electron configuration for Lithium is

$1s^2 2s^1$

- which reads "*one-ess-two, two-ess-one*"

Lecture 8 - Quantum Mechanical Model of the Periodic Table

The orbital diagrams can also be represented horizontally:
- Build up of period 1: H and He
- Build up of period 2: Li, Be, B, C, N, O, F and Ne
  - **Hund's rule:** *when orbital of equal energy are available, the election configuration of lowest energy has the maximum number of unpaired electrons with parallel spins.*

Lecture 8 - Quantum Mechanical Model of the Periodic Table

The orbital diagrams can also be represented horizontally:
- Build up of period 1: H and He
- Build up of period 2: Li, Be, B, C, N, O, F and Ne
- Build up of period 3:

Table 8.3 Partial Orbital Diagrams and Electron Configurations* for the Elements in Period 3

Atomic Number	Element	Partial Orbital Diagram (3s and 3p Sublevels Only) 3s	3p	Full Electron Configuration	Condensed Electron Configuration
11	Na	[↑]	[ ][ ][ ]	$[1s^2 2s^2 2p^6]\ 3s^1$	$[Ne]\ 3s^1$
12	Mg	[↑↓]	[ ][ ][ ]	$[1s^2 2s^2 2p^6]\ 3s^2$	$[Ne]\ 3s^2$
13	Al	[↑↓]	[↑][ ][ ]	$[1s^2 2s^2 2p^6]\ 3s^2 3p^1$	$[Ne]\ 3s^2 3p^1$
14	Si	[↑↓]	[↑][↑][ ]	$[1s^2 2s^2 2p^6]\ 3s^2 3p^2$	$[Ne]\ 3s^2 3p^2$
15	P	[↑↓]	[↑][↑][↑]	$[1s^2 2s^2 2p^6]\ 3s^2 3p^3$	$[Ne]\ 3s^2 3p^3$
16	S	[↑↓]	[↑↓][↑][↑]	$[1s^2 2s^2 2p^6]\ 3s^2 3p^4$	$[Ne]\ 3s^2 3p^4$
17	Cl	[↑↓]	[↑↓][↑↓][↑]	$[1s^2 2s^2 2p^6]\ 3s^2 3p^5$	$[Ne]\ 3s^2 3p^5$
18	Ar	[↑↓]	[↑↓][↑↓][↑↓]	$[1s^2 2s^2 2p^6]\ 3s^2 3p^6$	$[Ne]\ 3s^2 3p^6$

*Colored type indicates the sublevel to which the last electron is added.

Lecture 8 - Clicker Question 1

Given the partial (valence-level) orbital diagram:

2s	2p
[↑↓]	[↑↓][↑][↑]

What element is represent by this diagram

A) Carbon (C)
B) Oxygen (O)
C) Sulfur (S)
D) Nitrogen (N)

Lecture 8 - Quantum Mechanical Model of the Periodic Table

Electron configurations within groups.

- Members of the same group have similar outer electron configurations, which correlate with similar chemical behaviors.
- Orbitals are filled in order of increasing energy, which leads to outer electron configurations that recur *periodically*, which leads to chemical properties that recur *periodically*.

Lecture 8 - Quantum Mechanical Model of the Periodic Table

The orbital diagrams can also be represented horizontally:
- Build up of period 4:
  - First *d*-orbital transition series
  - The *3d* orbitals have an higher energy than the *4s* orbitals, and so are filled after the *4s* and before the *4p* orbitals.

Table 8.4 Partial Orbital Diagrams and Electron Configurations* for the Elements in Period 4

Atomic Number	Element	Partial Orbital Diagram (4s, 3d, and 4p Sublevels Only) 4s	3d	4p	Full Electron Configuration	Condensed Electron Configuration
19	K	[↑]	[ ][ ][ ][ ][ ]	[ ][ ][ ]	$[1s^22s^22p^63s^23p^6]\ 4s^1$	$[Ar]\ 4s^1$
20	Ca	[↑↓]	[ ][ ][ ][ ][ ]	[ ][ ][ ]	$[1s^22s^22p^63s^23p^6]\ 4s^2$	$[Ar]\ 4s^2$
21	Sc	[↑↓]	[↑][ ][ ][ ][ ]	[ ][ ][ ]	$[1s^22s^22p^63s^23p^6]\ 4s^23d^1$	$[Ar]\ 4s^23d^1$
22	Ti	[↑↓]	[↑][↑][ ][ ][ ]	[ ][ ][ ]	$[1s^22s^22p^63s^23p^6]\ 4s^23d^2$	$[Ar]\ 4s^23d^2$
23	V	[↑↓]	[↑][↑][↑][ ][ ]	[ ][ ][ ]	$[1s^22s^22p^63s^23p^6]\ 4s^23d^3$	$[Ar]\ 4s^23d^3$
24	Cr	[↑]	[↑][↑][↑][↑][↑]	[ ][ ][ ]	$[1s^22s^22p^63s^23p^6]\ 4s^13d^5$	$[Ar]\ 4s^13d^5$
25	Mn	[↑↓]	[↑][↑][↑][↑][↑]	[ ][ ][ ]	$[1s^22s^22p^63s^23p^6]\ 4s^23d^5$	$[Ar]\ 4s^23d^5$
26	Fe	[↑↓]	[↑↓][↑][↑][↑][↑]	[ ][ ][ ]	$[1s^22s^22p^63s^23p^6]\ 4s^23d^6$	$[Ar]\ 4s^23d^6$
27	Co	[↑↓]	[↑↓][↑↓][↑][↑][↑]	[ ][ ][ ]	$[1s^22s^22p^63s^23p^6]\ 4s^23d^7$	$[Ar]\ 4s^23d^7$
28	Ni	[↑↓]	[↑↓][↑↓][↑↓][↑][↑]	[ ][ ][ ]	$[1s^22s^22p^63s^23p^6]\ 4s^23d^8$	$[Ar]\ 4s^23d^8$
29	Cu	[↑]	[↑↓][↑↓][↑↓][↑↓][↑↓]	[ ][ ][ ]	$[1s^22s^22p^63s^23p^6]\ 4s^13d^{10}$	$[Ar]\ 4s^13d^{10}$
30	Zn	[↑↓]	[↑↓][↑↓][↑↓][↑↓][↑↓]	[ ][ ][ ]	$[1s^22s^22p^63s^23p^6]\ 4s^23d^{10}$	$[Ar]\ 4s^23d^{10}$
31	Ga	[↑↓]	[↑↓][↑↓][↑↓][↑↓][↑↓]	[↑][ ][ ]	$[1s^22s^22p^63s^23p^6]\ 4s^23d^{10}4p^1$	$[Ar]\ 4s^23d^{10}4p^1$
32	Ge	[↑↓]	[↑↓][↑↓][↑↓][↑↓][↑↓]	[↑][↑][ ]	$[1s^22s^22p^63s^23p^6]\ 4s^23d^{10}4p^2$	$[Ar]\ 4s^23d^{10}4p^2$
33	As	[↑↓]	[↑↓][↑↓][↑↓][↑↓][↑↓]	[↑][↑][↑]	$[1s^22s^22p^63s^23p^6]\ 4s^23d^{10}4p^3$	$[Ar]\ 4s^23d^{10}4p^3$
34	Se	[↑↓]	[↑↓][↑↓][↑↓][↑↓][↑↓]	[↑↓][↑][↑]	$[1s^22s^22p^63s^23p^6]\ 4s^23d^{10}4p^4$	$[Ar]\ 4s^23d^{10}4p^4$
35	Br	[↑↓]	[↑↓][↑↓][↑↓][↑↓][↑↓]	[↑↓][↑↓][↑]	$[1s^22s^22p^63s^23p^6]\ 4s^23d^{10}4p^5$	$[Ar]\ 4s^23d^{10}4p^5$
36	Kr	[↑↓]	[↑↓][↑↓][↑↓][↑↓][↑↓]	[↑↓][↑↓][↑↓]	$[1s^22s^22p^63s^23p^6]\ 4s^23d^{10}4p^6$	$[Ar]\ 4s^23d^{10}4p^6$

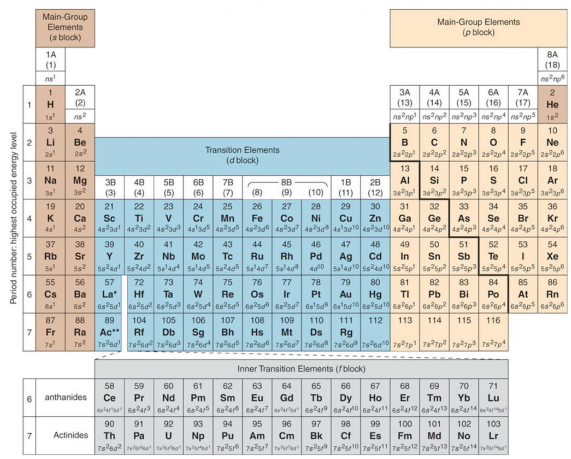
*Colored type indicates sublevel(s) whose occupancy changes when the last electron is added.

Lecture 8 - Quantum Mechanical Model of the Periodic Table

The orbital diagrams can also be represented horizontally:
- Build up of period 4:
  - First *d*-orbital transition series
  - The *3d* orbitals have an higher energy than the *4s* orbitals, and so are filled after the *4s* and before the *4p* orbitals.
  - Something interesting happens for Chromium (Z=24) and Copper (Z=29).
    - One of the *4s* electrons jumps into a *3d* orbital give either a filled or half-filled *3d* orbital.

Lecture 8 - Quantum Mechanical Model of the Periodic Table

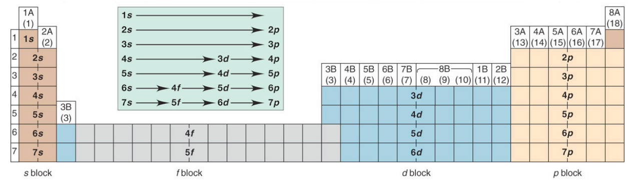
Groups have similar outer electron configurations:



Lecture 8 - Quantum Mechanical Model of the Periodic Table

Groups have similar outer electron configurations:

- Look where the last electron in the build-up process was placed.



Lecture 8 - Quantum Mechanical Model of the Periodic Table

Categories of electrons

- Inner (core) electrons.
  - Those found in the last noble gas (filled *s* and *p* orbitals)
- Outer electrons
  - Those found in the highest unfilled shell (*s* and *p* orbitals).
- Valence electrons
  - Those involved in forming compounds.
  - Among the **main group elements**, the valence electrons are the outer electrons.
  - Among the **transition elements**, the highest level *s* and *p* electrons (*ns* and *np*), plus, those in unfilled *(n-1)d* orbitals.

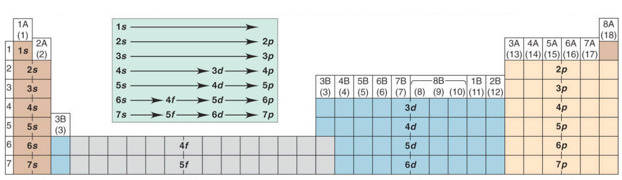
Lecture 8 - Quantum Mechanical Model of the Periodic Table

The orbital diagrams can also be represented horizontally:

- Build up of period 5:
  - First *f*-orbital inner transition series
  - The *4f* orbitals have a higher energy than the *5s* orbitals, and so are filled after the *5s* and before the *4d* orbitals.
  - The Actinide and Lanthanide series

Lecture 8 - Quantum Mechanical Model of the Periodic Table

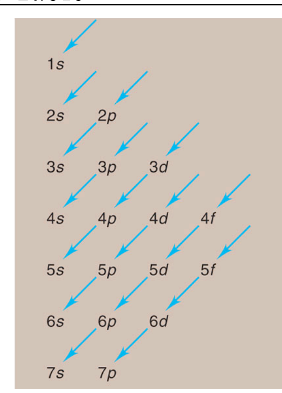
The periodic table can be used to figure out the order in which the electrons are placed in the build-up process:



Lecture 8 - Quantum Mechanical Model of the Periodic Table

The figure below also shows a mnemonic device that can be used to figure out the order in which the electrons are placed in the build-up process:

- The levels are listed from top to bottom.
- The sublevels for each level are listed from left to right.
- The filling order is obtained by moving diagonally from the upper-right to the lower-left, starting from the left.



Lecture 8 - Clicker Question 5

Which of the following condensed notations gives the ground state electronic configuration for calcium (Ca)?

A) $1s^2 2s^2 2p^6 3s^2$

B) $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$

C) $1s^2 2s^2 2p^6 3s^2 3p^6$

D) $1s^2 2s^2 2p^6 3s^2 3p^6 3d^2$

Lecture 8 - Clicker Question 5

Which of the following condensed notations gives the ground state electronic configuration for nickel (Ni)?

A) $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^8$

B) $1s^2 2s^2 2p^6 3s^2 3p^6 4s^1 3d^9$

C) $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10}$

D) $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^4$

Lecture 8 - Clicker Question 5

Which of the following condensed notations gives the ground state electronic configuration for molybdenum (Mo)?

A) $1s^2 2s^2 2p^6 3s^2$

B) $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^4$

C) $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^1 4d^5$

D) $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^4$

Lecture 8 - Clicker Question 2

How many inner electrons are present in an atom of Fe?

A) 10

B) 8

C) 18

D) 36

E) 2

Lecture 8 - Clicker Question 3

How many outer electrons are present in an atom of Fe?

A) 10

B) 8

C) 18

D) 36

E) 2

Lecture 8 - Clicker Question 4

How many valence electrons are present in an atom of Fe?

A) 10

B) 8

C) 18

D) 36

E) 2

Unit II - Up Next

Unit II - The Elements and the Structure of Their Atoms

- The periodic trends observed for three key properties of the elements
- How the electronic structure of the elements affects their chemical reactivity.

The End