



# **Welcome to Chemistry 154!**

**Chemistry for Engineering**



## Reminders

- **Worksheet: Unit 2**
- Due September 18<sup>th</sup> at 11:59pm
- **Achieve Assignment #1**
- Due September 13<sup>th</sup> at 11:59pm
- **Canvas Bonus Assignment**
- Due September 13<sup>th</sup> at 11:59pm

Worksheet →  
All Lectures Canvas Site  
Submission link →  
Section 113 Canvas Site

All Lectures Canvas Site

## Instructor Office Hours

Monday and Friday 7-8pm via Zoom (All Lectures Site)

# **Unit 2**

## **Atomic Structure and Properties & Chemical Bonding**

# Learning Objectives

After mastering this unit you will be able to:

- Define the terms valence and core electrons
- Determine the number of valence electrons and core electrons based on electron configuration for atoms and ions
- Define, in words or using equations, effective nuclear charge ( $Z_{\text{eff}}$ ), atomic and ionic radius, ionization energy, and electron affinity.
- Rank elements and ions according to their  $Z_{\text{eff}}$ , atomic size, ionization energy, and electron affinity.
- Rationalize the periodic trends of radii, relative ionization energies and electron affinities of atoms and ions based on nuclear charge and/or electron configurations.

# Learning Objectives (continued)

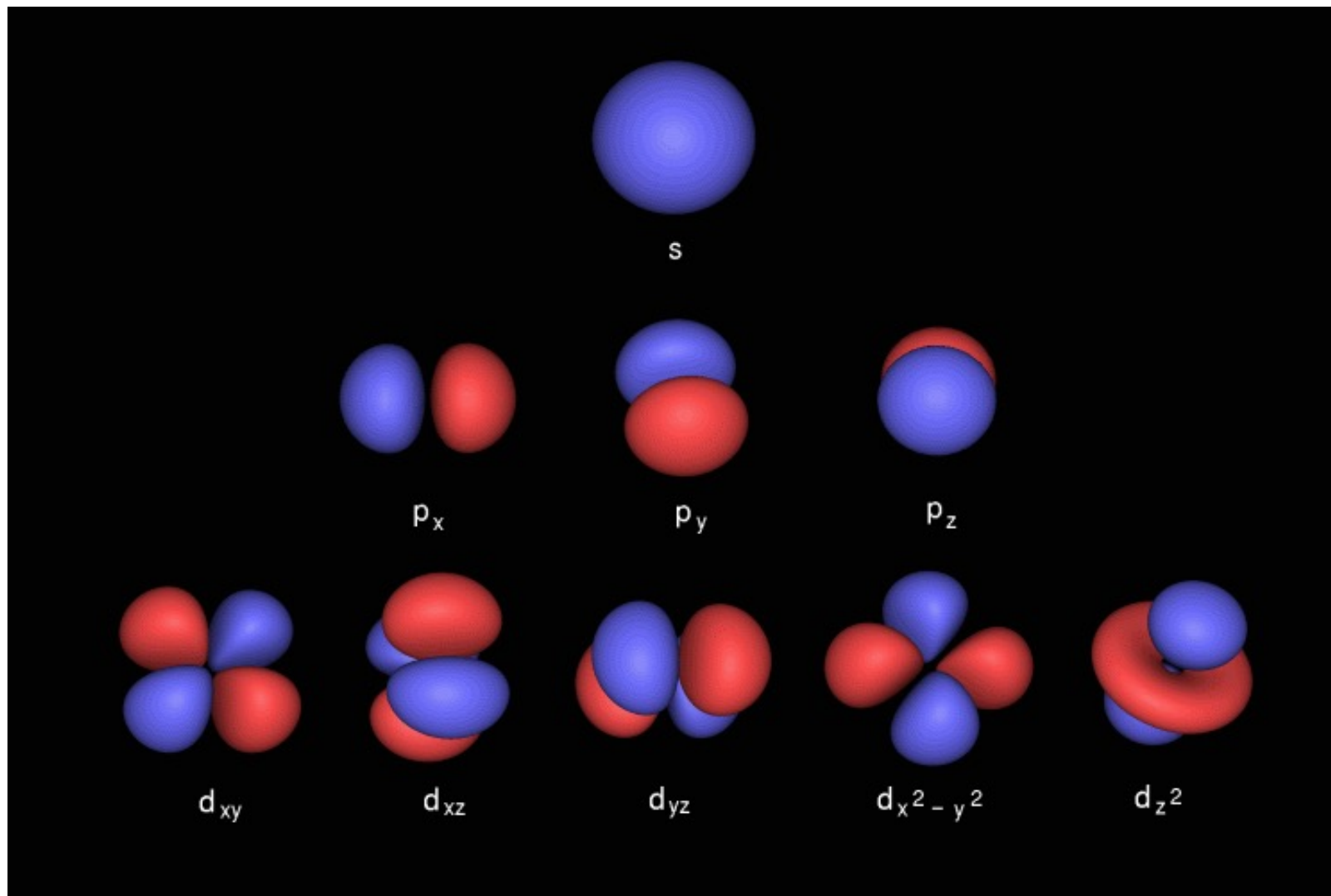
- Describe the nature of ionic and covalent bonds.
- Define electronegativity and describe how electronegativity varies with position in the periodic table.
- Predict the nature of a chemical bond (ionic/covalent, polar/nonpolar) and justify your prediction by comparing the relative electronegativities of the atoms involved.
- Predict lattice energy trends in ionic solids & justify your predictions.

# Salient Features of Quantum Mechanics

Small objects, like electrons, behave as both particles and waves which means they can interfere, diffract and spread. Orbitals give the probability for finding electrons at particular points in space.

Quantum mechanics is the theory explaining why energies and angular momenta of atoms and molecules are quantized, that is only have certain discrete values.

# Hydrogenic Orbitals



# Quantum Numbers

Quantum Number		Values	Example
$n$	<i>Principal Quantum Number</i>	Positive integer values	1, 2, 3, ...
$\ell$	<i>Angular Momentum Quantum Number</i>	Integer values $0 \leq \ell \leq n-1$	0, 1 (if $n=2$ )
$m_\ell$	<i>Magnetic Quantum Number</i>	Integer values $-\ell \leq m_\ell \leq \ell$	-1, 0, 1 (if $\ell = 1$ )

$\ell=0$ , indicates *s* subshell  
 $\ell=1$ , indicates *p* subshell  
 $\ell=2$ , indicates *d* subshell  
 $\ell=3$ , indicates *f* subshell

**Note:** This slide is **Additional information**. It is meant to help you understand “max. # of electrons in subshells” determination.

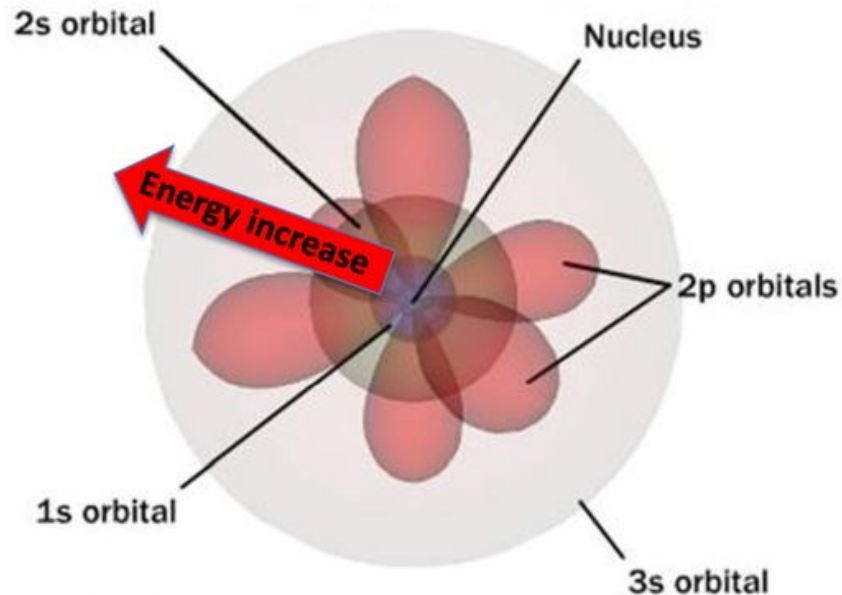


# Shells and subshells

Shell (n)	Sub-shells	Max. # e <sup>-</sup> in subshells	
1	s	2	$2(1)^2 = 2$
2	s, p	$2 + 6 = 8$	$2(2)^2 = 8$
3	s, p, d	$2 + 6 + 10 = 18$	$2(3)^2 = 18$
4	s, p, d, f	$2 + 6 + 10 + 14 = 32$	$2(4)^2 = 32$

# Shell Structure of Atoms

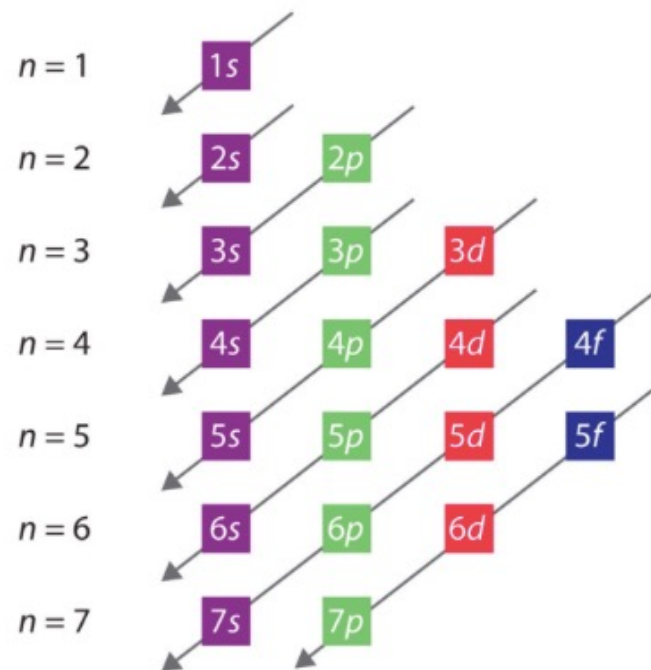
Orbitals become larger as the energy level increases



- **Electrons filling order : 1s, 2s 2p, 3s**
- **Orbitals arranged in order of increasing energy: 1s, 2s 2p, 3s**
- **Orbitals arranged in increasing size: (smallest) 1s < 2s < 2p < 3s (largest)**

# Orbital Filling

- **Aufbau Principle**
- Fill orbitals with electrons from lowest energy first
- **Pauli Exclusion Principle**
- Each orbital holds no more than two electrons
- The two electrons in an orbital must have opposite spins
- **Hund's Rule**
- Electrons occupy orbitals of identical energy singly first (with parallel spins) before being paired up in an orbital



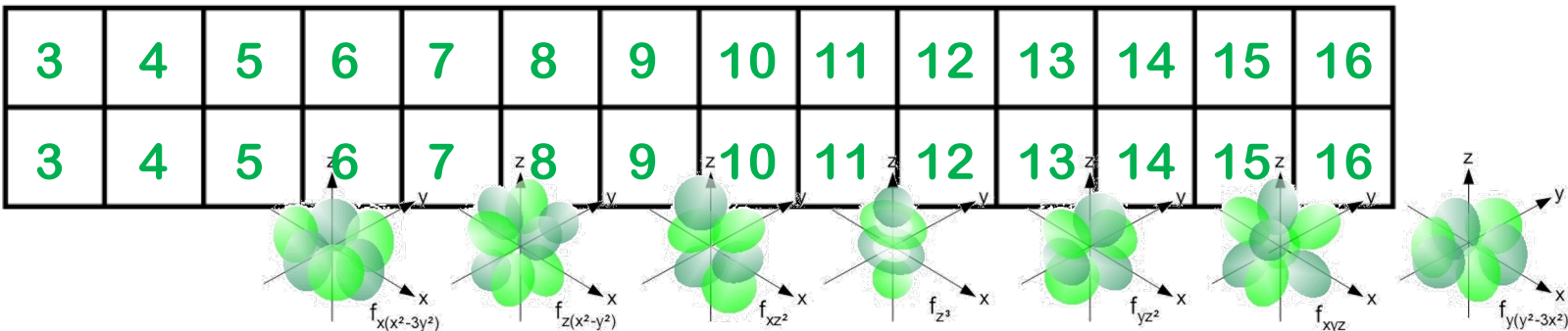
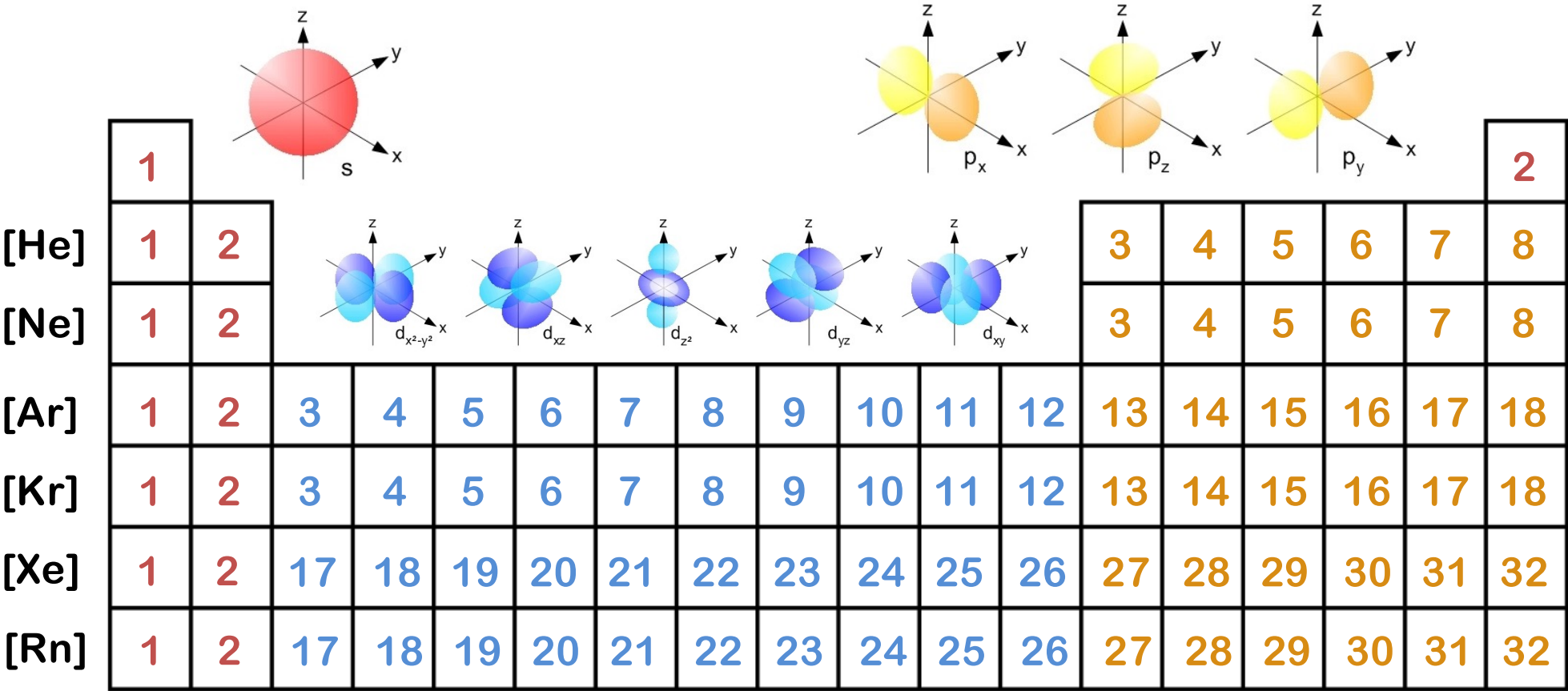
# Electronic Structure

Electrons have negative charge but are also tiny magnets. Spin is our way of describing the orientation of the poles of these magnets (“spin up  $\uparrow$ ” or “spin down  $\downarrow$ ”).

The Pauli Principle states a maximum of 2 electrons can be assigned to any one orbital, and the electrons must have opposite spins ( $\uparrow\downarrow$ ).

Orbitals are arranged in shells, labelled by  $n$ , and sub-shells. Each shell contains only certain orbitals. Starting with the lowest shell,  $n=1$ , electrons are assigned to s, p, d orbitals until they are all accounted for. Note: orbitals get bigger as  $n$  increases (a 2s orbital is bigger than a 1s orbital) thus forming the shell structure of atoms.

## Fill in electrons



# Valence Electrons

## For elements in the s- and p-blocks only

The electrons occupying the  $s$  and  $p$  subshells with the largest  $n$  (for the neutral element) are called valence electrons, and the collection of occupied subshells is called the valence shell.

Electrons which aren't valence electrons are called core electrons.

In solids, valence orbitals on atoms overlap to form valence bands extending throughout the material.

Valence electrons are fundamental to chemistry because they are involved in the formation of bonds. Core electrons are not involved in chemical bonding.

# Valence electrons for neutral elements

Diagram illustrating the 'EXCEPTION' rule. A grid of numbers 1 through 8 is shown. The number 1 is in the top-left cell, and the number 2 is in the top-right cell. A red arrow points from the word 'EXCEPTION' to the number 2, indicating that the number 2 is the exception to the rule.

# Clicker Question

How many valence electrons does Li have?

a) 0

☒ b) 1

c) 2

d) 8

e) 4



# Clicker Question

How many valence electrons does  $\text{Li}^+$  have?

- a) 0
- b) 1
- c) 2
- d) 8
- e) 4

## Worksheet Question #2

Write the electron configurations for the following chemical species:

a) P      $[\text{Ne}]3s^23p^3$

b)  $\text{S}^{2-}$       $[\text{Ne}]3s^23p^6$  or  $[\text{Ar}]$

c) Se

d)  $\text{Mg}^+$

e) In

} Please complete these yourself

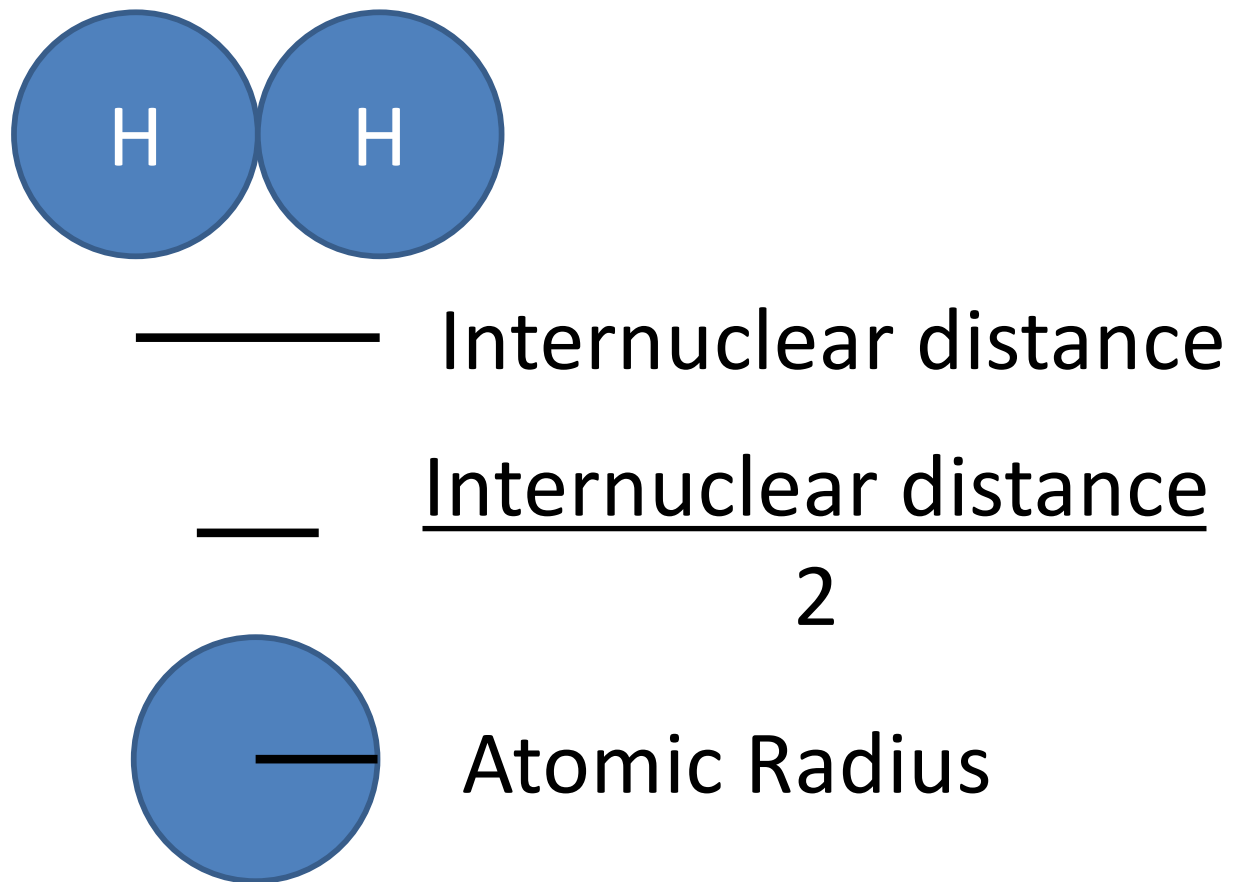
In-class example:

Electronic configuration of **Ga**:  $[\text{Ar}]4s^23d^{10}4p^1$

# Periodic Properties

- Atomic radius
- Effective nuclear charge ( $Z_{\text{eff}}$ )
- Ionization energy
- Electron affinity
- Electronegativity (EN)

# Atomic Radius



Atomic radius is calculated by measuring the internuclear distance and dividing by 2

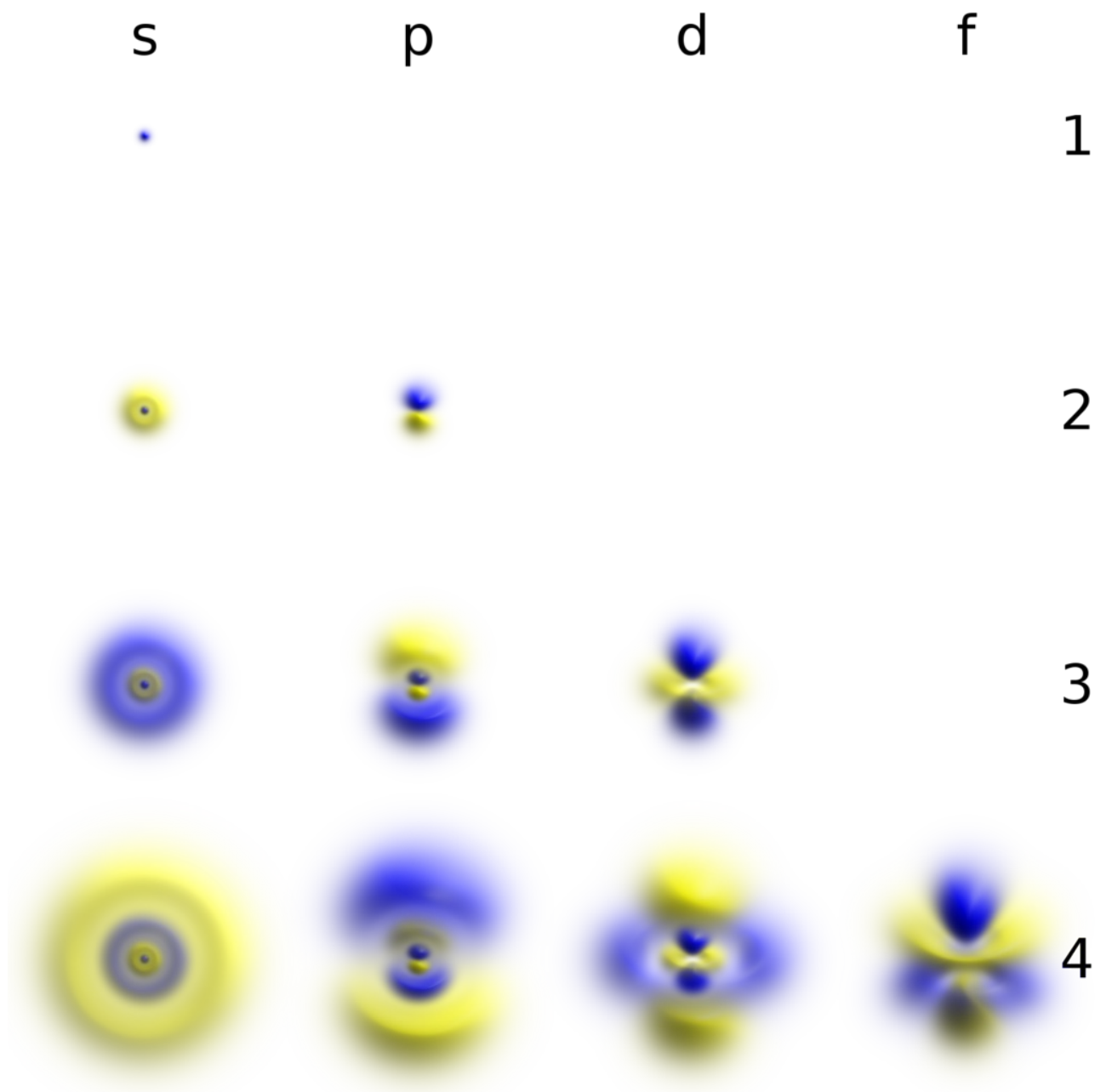
# Atomic Radius (across a period)

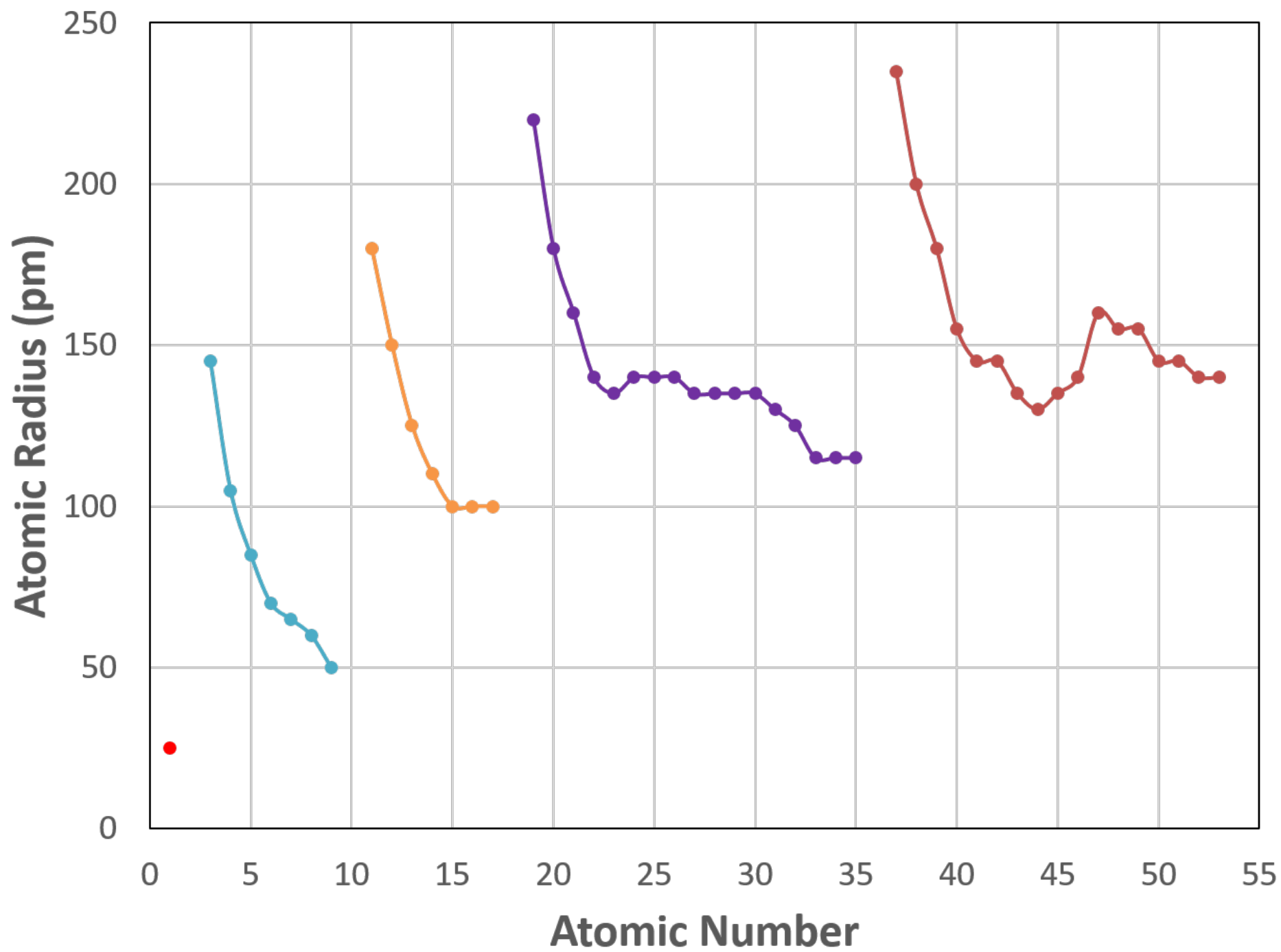
Element	Radius (Å)
Be	0.96
B	0.84
C	0.76
N	0.71
O	0.66
F	0.57
Ne	n/a

# Atomic radius (down a group)

Element	Radius (Å)
Li	1.28
Na	1.66
K	2.03
Rb	2.20
Cs	2.44
Fr	n/a

# Relative Orbital Sizes

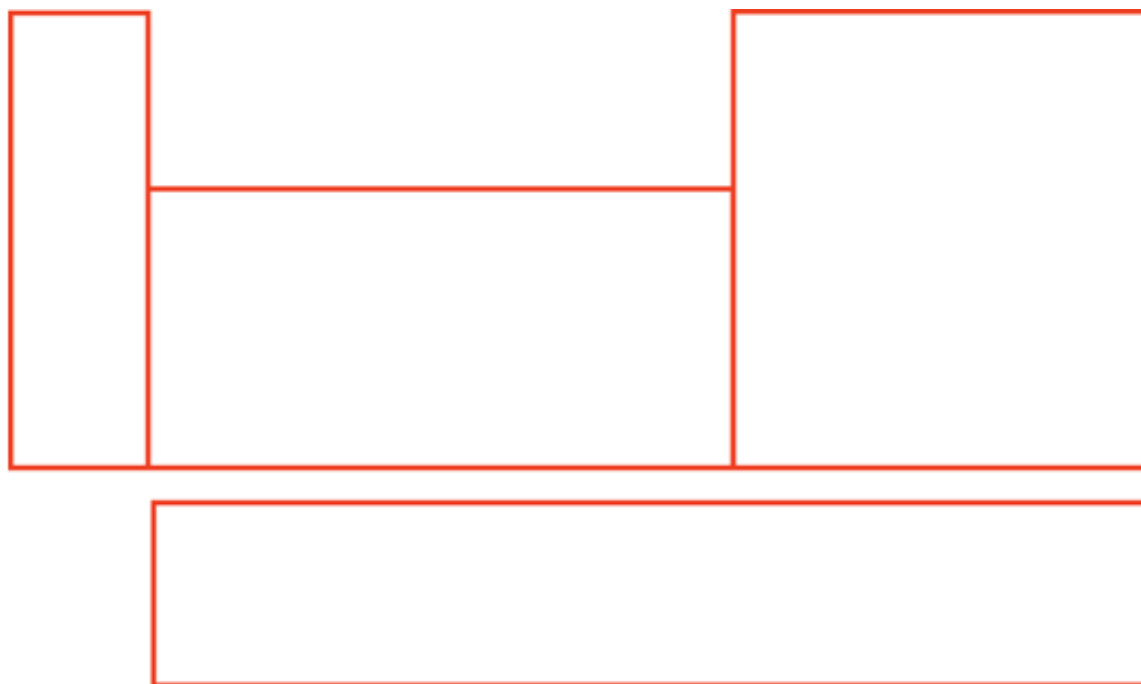






# Homework: Worksheet Question #3

Draw arrows to explain the trends of  $Z_{\text{eff}}$  and size on the periodic table below.



# Homework: Worksheet Question #4

Calculate the atomic radius of silicon (one of the most important elements in the microelectronics industry), given the following information:

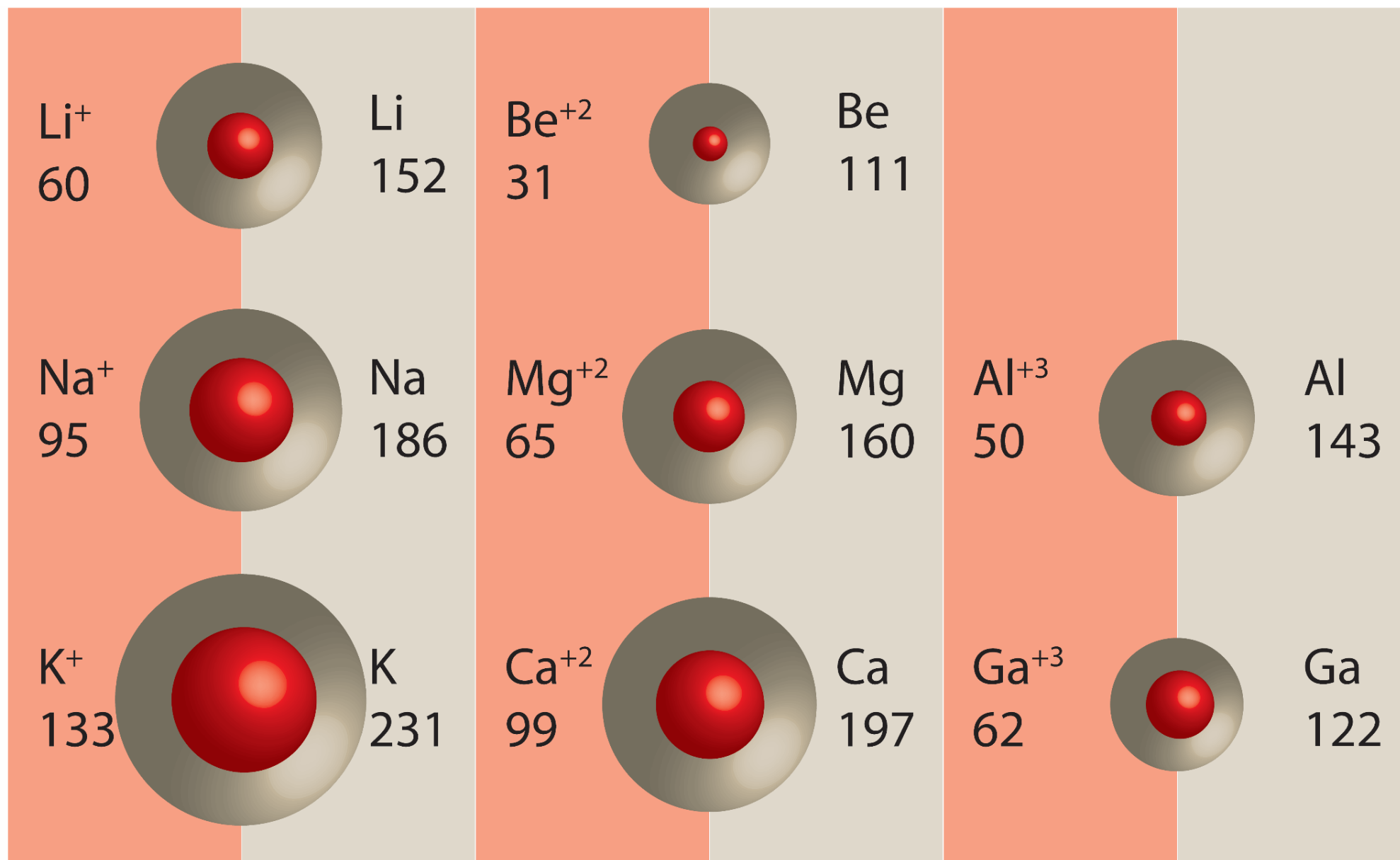
- the H-H bond distance in  $\text{H}_2$  is  $0.74 \text{ \AA}$
- the Si-H bond distance in  $\text{SiH}_4$  is  $1.46 \text{ \AA}$

**Remember**  $1 \text{ \AA} = 1 \times 10^{-10} \text{ m}$



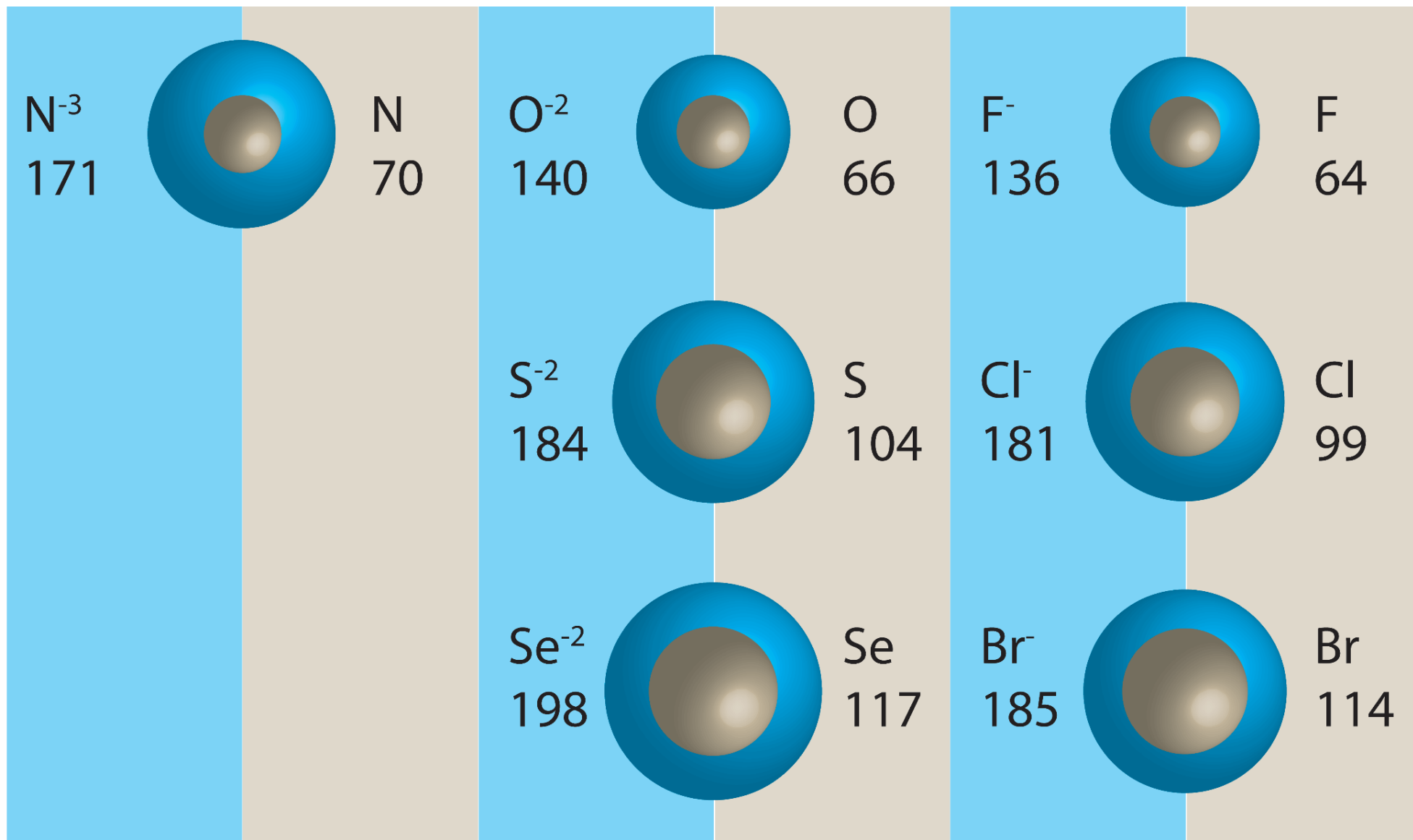
# Cationic radii

For a given atom, its cation is always smaller than the neutral species.



# Anionic radii

For a given atom, its anion is always larger than the neutral species.



## Worksheet Question #5

Rationalize the difference in the atomic and ionic radii of the following species:

(a) Se (117 pm) and  $\text{Se}^{2-}$  (198 pm)

(b) K (231 pm) and  $\text{K}^+$  (133 pm)

# Isoelectronic species

Atoms and ions with the same number of electrons are said to be *isoelectronic*. In a set of isoelectronic species, the most negative species has the largest radius.

$\text{K}^+$

Ar

$\text{Cl}^-$



Increasing Atomic or Ionic Radius

## Clicker Question

Which of the following isoelectronic species is expected to have the largest radius?

a.  $\text{O}^{2-}$

b.  $\text{N}^{3-}$

c.  $\text{Na}^+$

d.  $\text{F}^-$

# Effective nuclear charge ( $Z_{\text{eff}}$ )

Coulomb's Law

$$E \propto \frac{q^{(+)}q^{(-)}}{r}$$

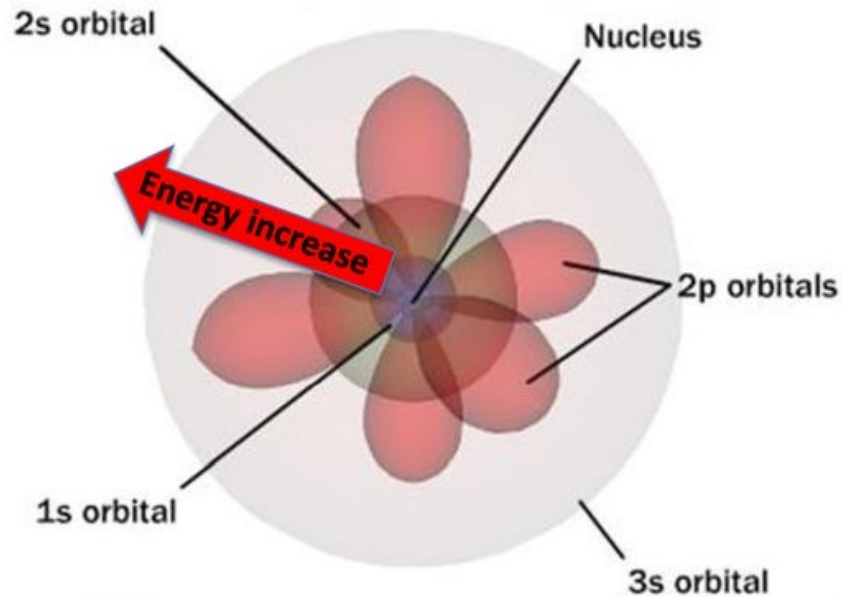
Core electrons are close to the nucleus and effectively screen some of its positive charge from valence electrons further away. Valence electrons also partially screen each other from the nuclear charge. Thus, a valence electron “feels” an effective nuclear charge ( $Z_{\text{eff}}$ ) that is less than the actual nuclear charge  $Z$ .

Note:  $Z_{\text{eff}}$  is a theoretically calculated property.



# Shell Structure of Atoms

Orbitals become larger as the energy level increases



- **Electrons filling order : 1s, 2s 2p, 3s**
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- **Orbitals arranged in increasing size: (smallest) 1s < 2s < 2p < 3s (largest)**

# Effective nuclear charge ( $Z_{\text{eff}}$ )

