THE SHAPES OF THE ATOMIC ORBITALS:

Atomic orbital is a region of space where electrons can be located. The shapes are uncertain, but predictions have been made by experimentation. Another difficult task is describing where an electron is. We can think of it as a wave, and describing its exact location is impossible for us to comprehend. Instead, we can think of it as the statistical probability of the electron being found at a particular place. An electron cloud is used for showing the probability of where an electron is using a dot-density diagram. The denser the dots are in the diagram, the more probability that an electron could be found there.

1. *s* orbitals have a spherical shell shape and the faint dark blue circle represents in cross-section, the region of maximum electron density.
2. *p* orbitals have two lobes extending out into three dimensional space. Since there are 3 *p* orbitals per energy level, the lobes extend out along the *x*-axis (p_x orbital), the *y*-axis (p_y orbital), and the *z*-axis (p_z orbital) at 90^o to each other.
3. The *d* orbital's shapes are even more complex because there are 5 orbitals in a d subshell. Four of the five *d* orbitals (d_{xy}, d_{xz}, d_{yz}, and $d_{x^2-y^2}$) have four lobes extending out perpendicular to each other. The last one, d_{z^2}, has two lobes extending out along the *z*-axis with a torus (doughnut-shaped ring) around the center on the *x*-*y* plane.

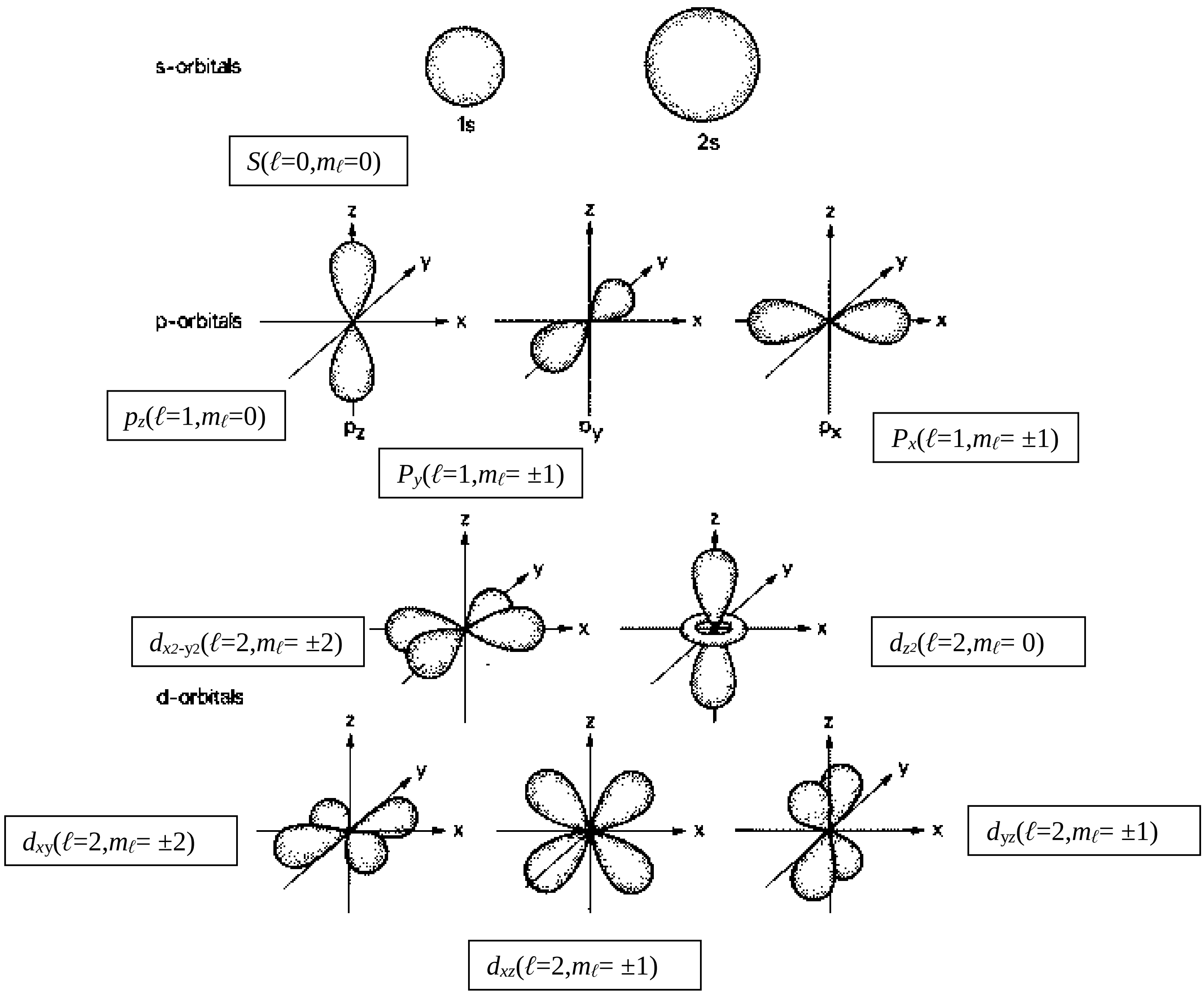

Fig (1).Boundary surface diagrams for *s*,*p*. and *d* atomic orbitals.

IONIZATION ENERGY:

The **ionization energy** (**IE**) of an atom or molecule describes the minimum amount of energy required to remove an electron (to infinity) from the atom or molecule in the gaseous state.

$$X + \text{energy} \rightarrow X^+ + e^-$$

The units for ionization energy vary from discipline to discipline**.**

In physics, the ionization energy is typically specified in **electron volts** (eV) and refers to the energy required to remove a single electron from a single atom or molecule.

In chemistry, the ionization energy is typically specified as a molar quantity (molar ionization energy) and is reported in units of **kJ/mol** (the amount of energy it takes for all the atoms in a mole to lose one electron each),(Conversion factor from *eV to kJ / mol is (electron volt to kilojoule) / mole =* $6.24150913 \times 10^{21}$ mol^{-1} *)* .

For example, the first ionization energy of hydrogen is 13.6 eV.

When considering an initially neutral atom, expelling the first electron will require less energy than expelling the second, the second will require less energy than the third, and so on. Each successive electron requires more energy to be released. This is because after the first electron is lost, the overall charge of the atom becomes positive, and the negative forces of the electron will be attracted to the positive charge of the newly formed ion. The more electrons that are lost, the more positive this ion will be, the harder it is to separate the electrons from the atom.

For example, Lithium atom with the electronic configuration $1s^2\,2s^1$ has three ionization energies:

1st ionization energy	$Li \rightarrow Li^+ + e^-_{2s}$	$IE_1 = 5.39eV$
2nd ionization energy	$Li^+ \rightarrow Li^{2+} + e^-_{1s}$	$IE_2 = 75.62$ eV
3rd ionization energy	$Li^{2+} \rightarrow Li^{3+} + e^-_{1s}$	$IE_3 = 122.42$ eV

This means that $IE_1 < IE_2 < IE_3 < ... < IE_n$ will always be true.

In general, (see table (4)) the further away an electron is from the nucleus, the easier it is for it to be expelled. In other words, ionization energy is a function of atomic radius; the larger the radius, the smaller the amount of energy required to remove the electron from the outer most orbital.

Table (4): See first, second, and third ionization energies of elements/ions in the table below

Ionization Energies (kJ/mol)

	1	2	3	4	5	6	7	8
H	1312							
He	2372	5250						
Li	520	7297	11810					
Be	899	1757	14845	21000				
B	800	2426	3659	25020	32820			
C	1086	2352	4619	6221	37820	47260		
N	1402	2855	4576	7473	9442	53250	64340	
O	1314	3388	5296	7467	10987	13320	71320	84070
F	1680	3375	6045	8408	11020	15160	17860	92010
Ne	2080	3963	6130	9361	12180	15240		
Na	496	4563	6913	9541	13350	16600	20113	25666
Mg	737	1450	7731	10545	13627	17995	21700	25662

Factors affecting the ionization energy are:

1. **Atomic size:** In small atoms electrons remains closer to nucleus and they feel more nuclear attraction, so more ionization energy is required to remove an electron from small atoms. While in big sized atoms, valence electrons are away from nucleus, so they experience less nuclear attraction. Hence it requires less ionization energy to remove electrons from big atoms. **Therefore, Ionization energy is inversely proportional to Atomic size.**

2. **Nuclear charge:** By increasing the nuclear charge electrons feel more nuclear attraction. Hence more ionization energy is required. **Therefore, Ionization Energy is directly proportional to Nuclear charge.**

3. **Orbital penetration (penetration power):** It's easier to remove electrons from *p* orbitals than from *s* orbitals, because the *s* orbitals penetrate towards the nucleus more closely than the *p* orbitals, thus making the electrons in the *s* orbital feel

greater nuclear attraction. The order of penetration power of different subshells is: s > p > d > f.

Therefore, Ionization energy is directly proportional to Penetration Power.

4. **Electron pairing (Stability):** within a subshell, paired electrons are easier to remove than unpaired ones. This is because repulsion between electrons in the same orbital is higher than repulsion between electrons in different orbitals. Therefore, Ionization energy is directly proportional to Stability. Ionization Energy is more of full-filled shell as compared to half-filled shell.

5. Screening & Shielding effect: Presence of other orbits between nucleus and last orbit decreases the nuclear attraction. This effect is called screening effect but electron-electron repulsion is called shielding effect which also decreases the nuclear attraction. Due to presence of these effects ionization energy decreases.