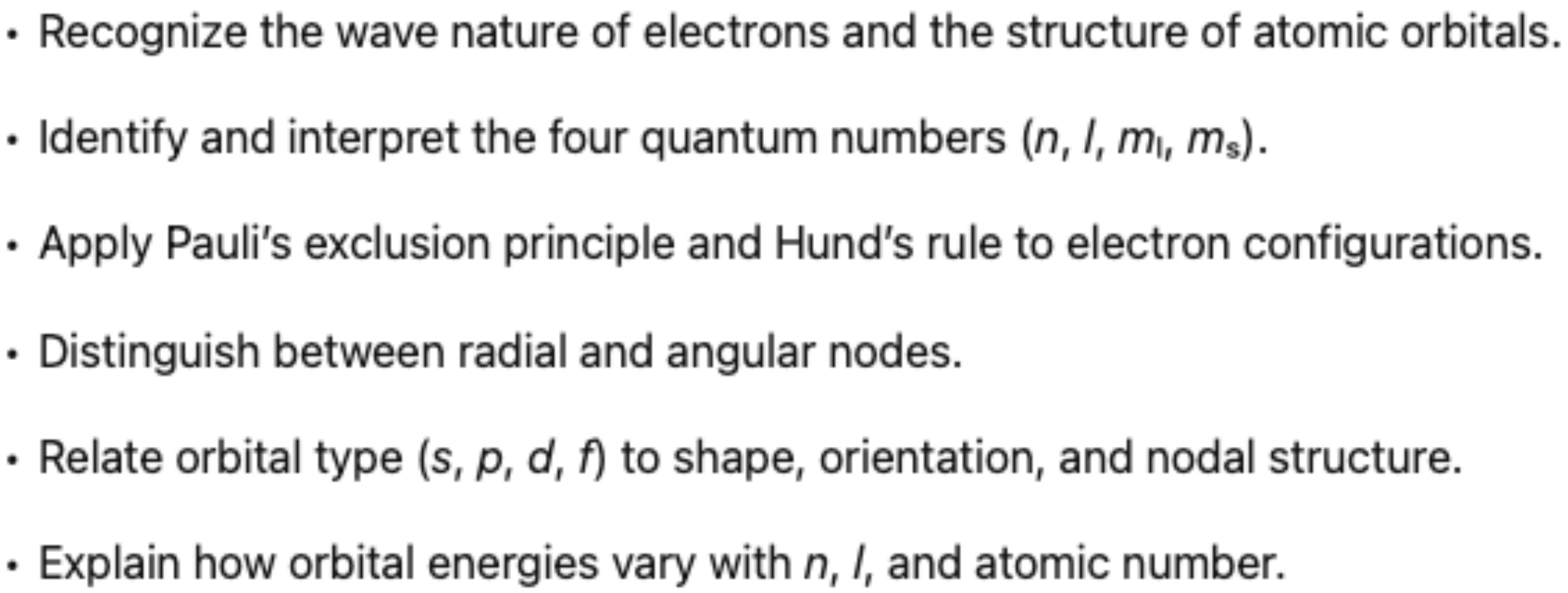
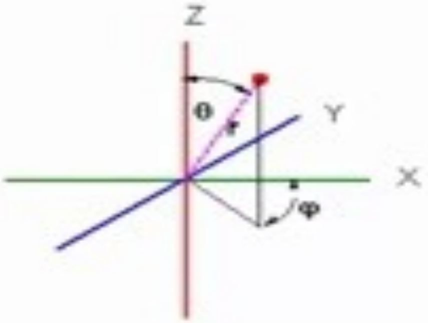
Atomic Orbitals



- Recognize the wave nature of electrons and the structure of atomic orbitals.
- Identify and interpret the four quantum numbers (n, l, m_l, m_s).
- Apply Pauli's exclusion principle and Hund's rule to electron configurations.
- Distinguish between radial and angular nodes.
- Relate orbital type (*s*, *p*, *d*, *f*) to shape, orientation, and nodal structure.
- Explain how orbital energies vary with n, l, and atomic number.

Orbital Wavefunctions



$$\Psi_{n,l,m_l} = \underbrace{R_{n,l}(r)}_{\text{Radial part}}\underbrace{Y_{l,m_l}(\theta,\varphi)}_{\text{Angular part}}$$

Radial part: Defines the size of the orbital

Angular part: Defines the shape of the orbital

Quantum Numbers

Principle quantum # (n = 1,2,3,...)

Largely defines the size and energy of the orbital

Orbital angular momentum quantum # (ℓ = 0, 1, ... $n-1$)

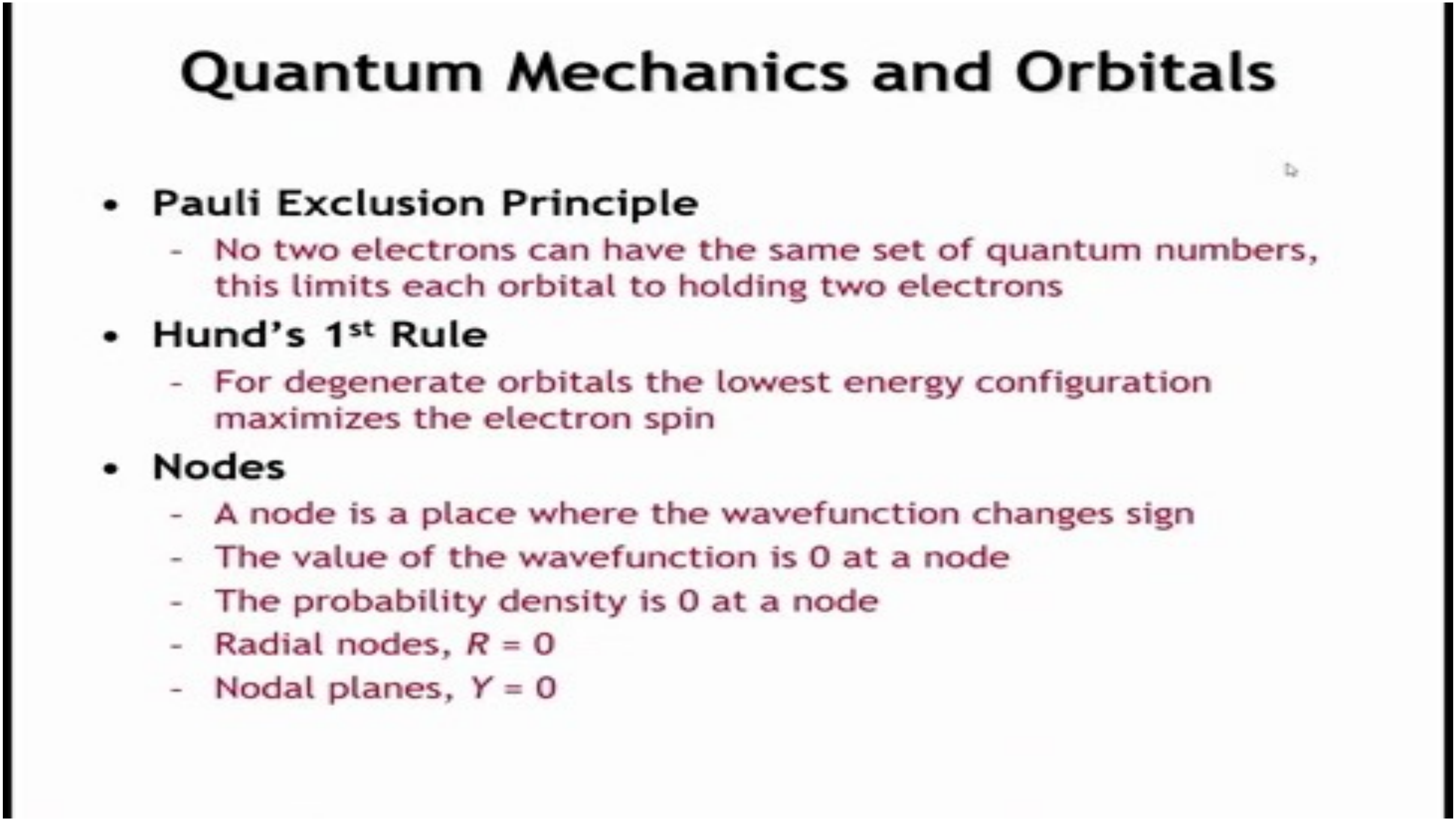
Defines the shape of the orbital

Magnetic quantum # ($m_\ell = -\ell$ to ℓ)

Defines the orientation of the orbital

Spin quantum # ($m_s = +½, -½$)

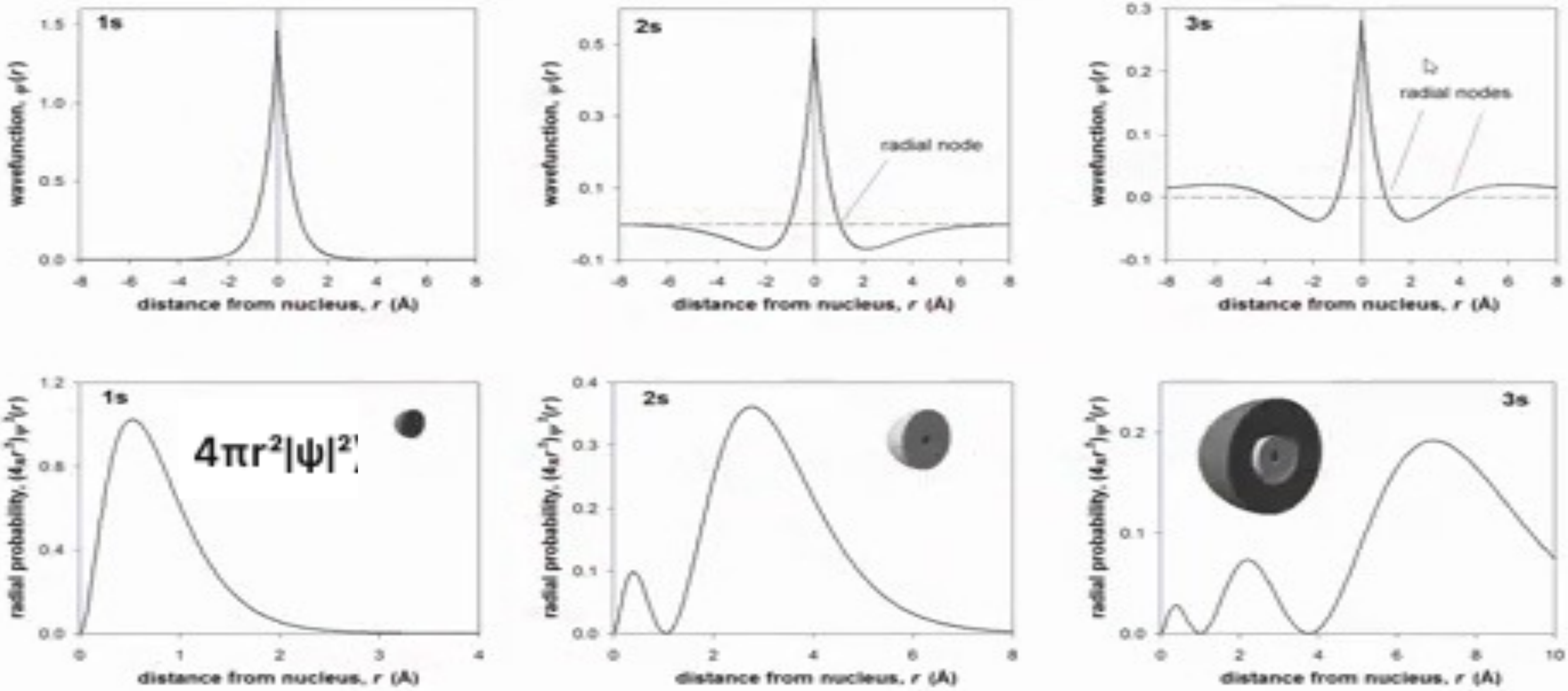
Defines the spin of the electron



Quantum Mechanics and Orbitals

- **Pauli Exclusion Principle**
  - No two electrons can have the same set of quantum numbers, this limits each orbital to holding two electrons
- **Hund's 1st Rule**
  - For degenerate orbitals the lowest energy configuration maximizes the electron spin
- **Nodes**
  - A node is a place where the wavefunction changes sign
  - The value of the wavefunction is 0 at a node
  - The probability density is 0 at a node
  - Radial nodes, $R = 0$
  - Nodal planes, $Y = 0$

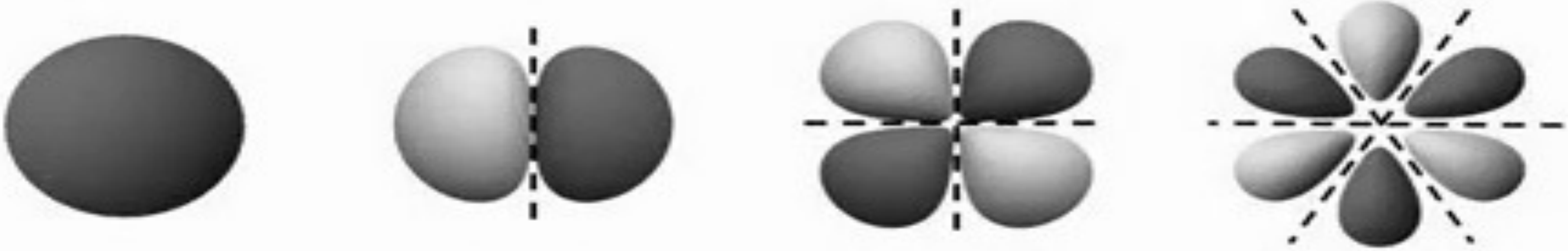
Principle Quantum # and Radial Nodes



The number of radial nodes is equal to n – ℓ – 1

These impact the energy of the orbital

Orbital Angular Momentum Quantum # and Nodal Planes



s orbital
($\ell = 0$)

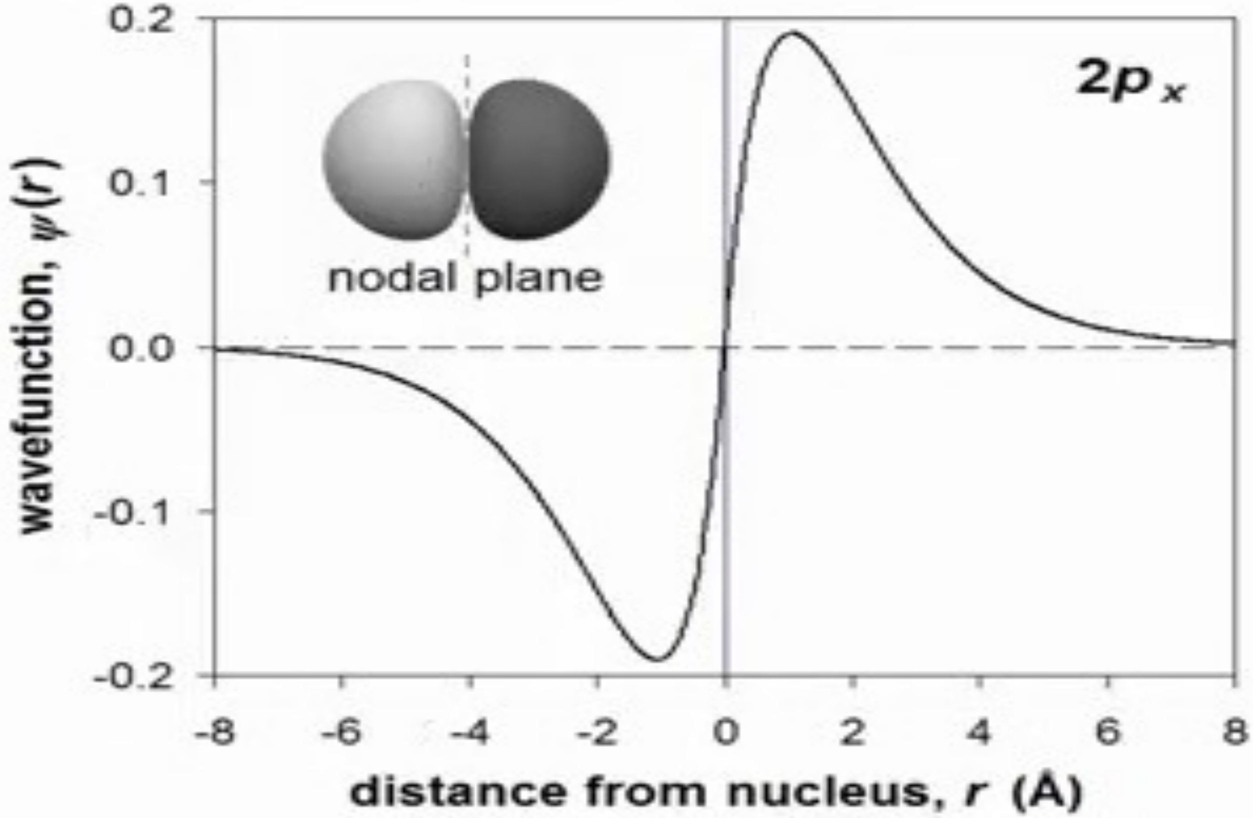
p orbital
($\ell = 1$)

d orbital
($\ell = 2$)

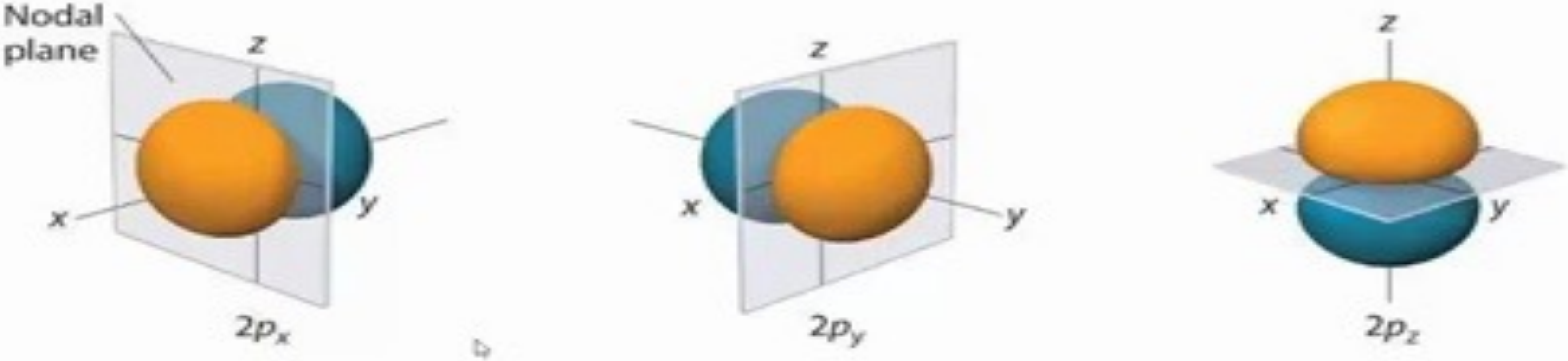
f orbital
($\ell = 3$)

The number of nodal planes is equal to ℓ
These impact the shape of the orbital

A closer look at the wavefunction



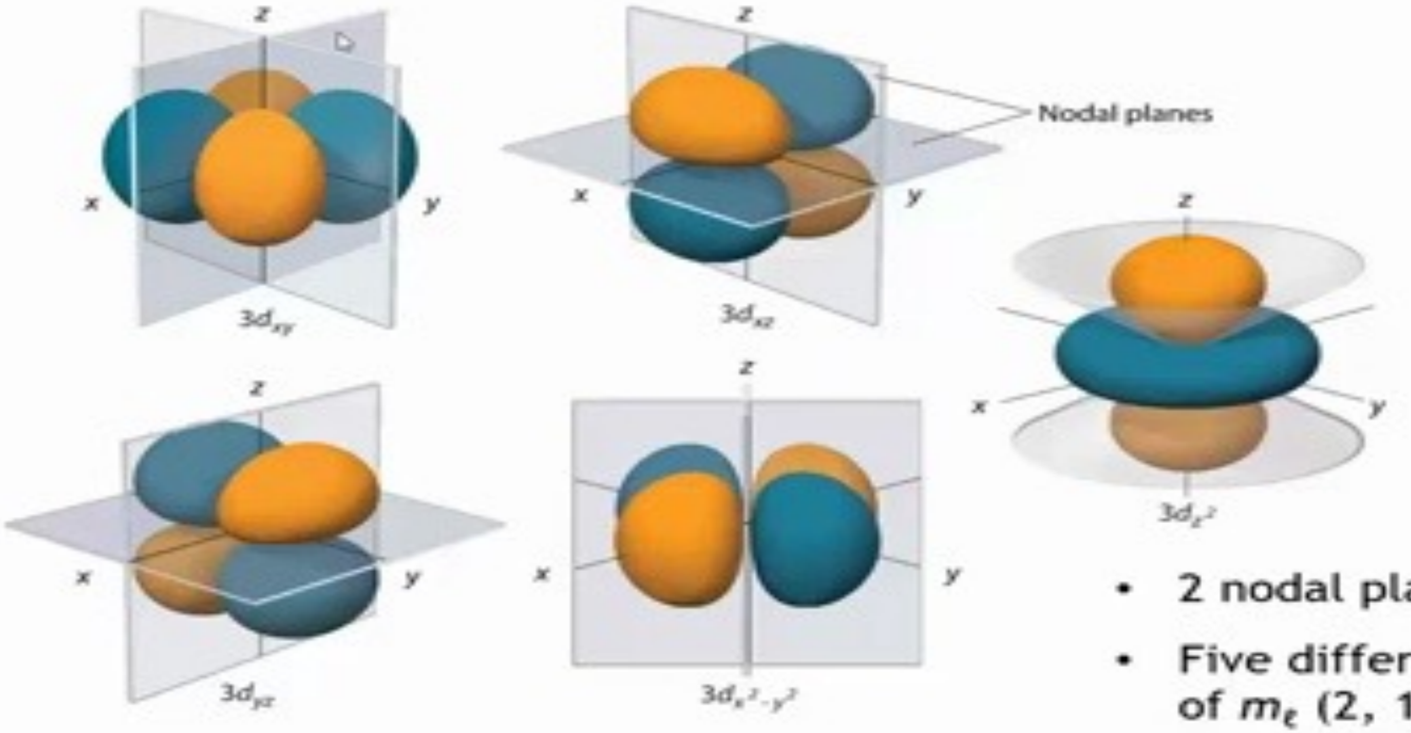
Orbital Shapes – p orbitals



- 1 nodal plane
- Three different values of m_ℓ (1, 0, −1) each leading to a different orientation (p_x, p_y, p_z)

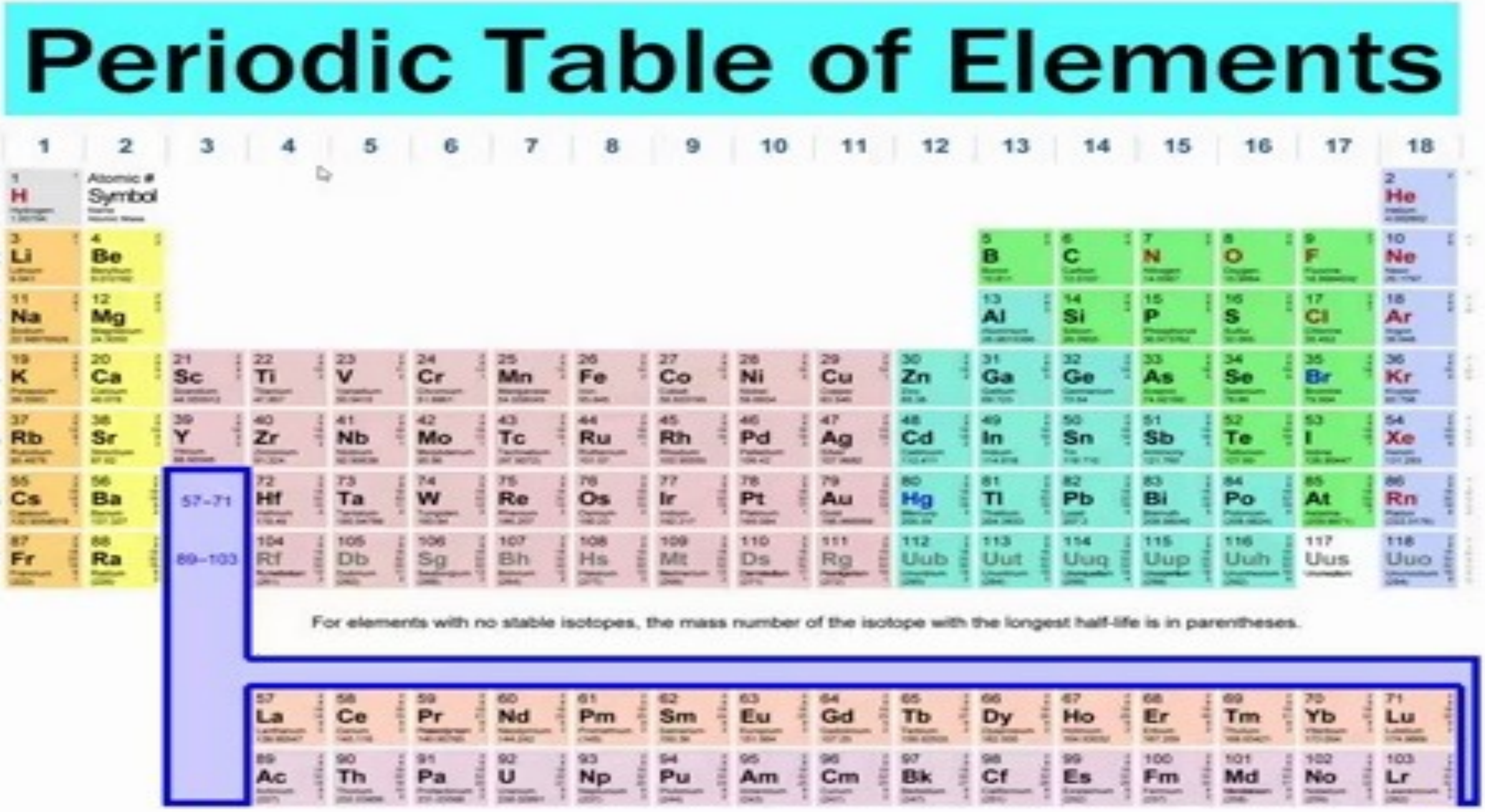
Image taken from:
https://saylordotorg.github.io/text_general-chemistry-principles-patterns-and-applications-v1.0/s10-05-atomic-orbitals-and-their-ener.html

Orbital Shapes – d orbitals



- 2 nodal planes
- Five different values of m_ℓ (2, 1, 0, −1, −2)

Image taken from:
https://saylordotorg.github.io/text_general-chemistry-principles-patterns-and-applications-v1.0/s10-05-atomic-orbitals-and-their-ener.html



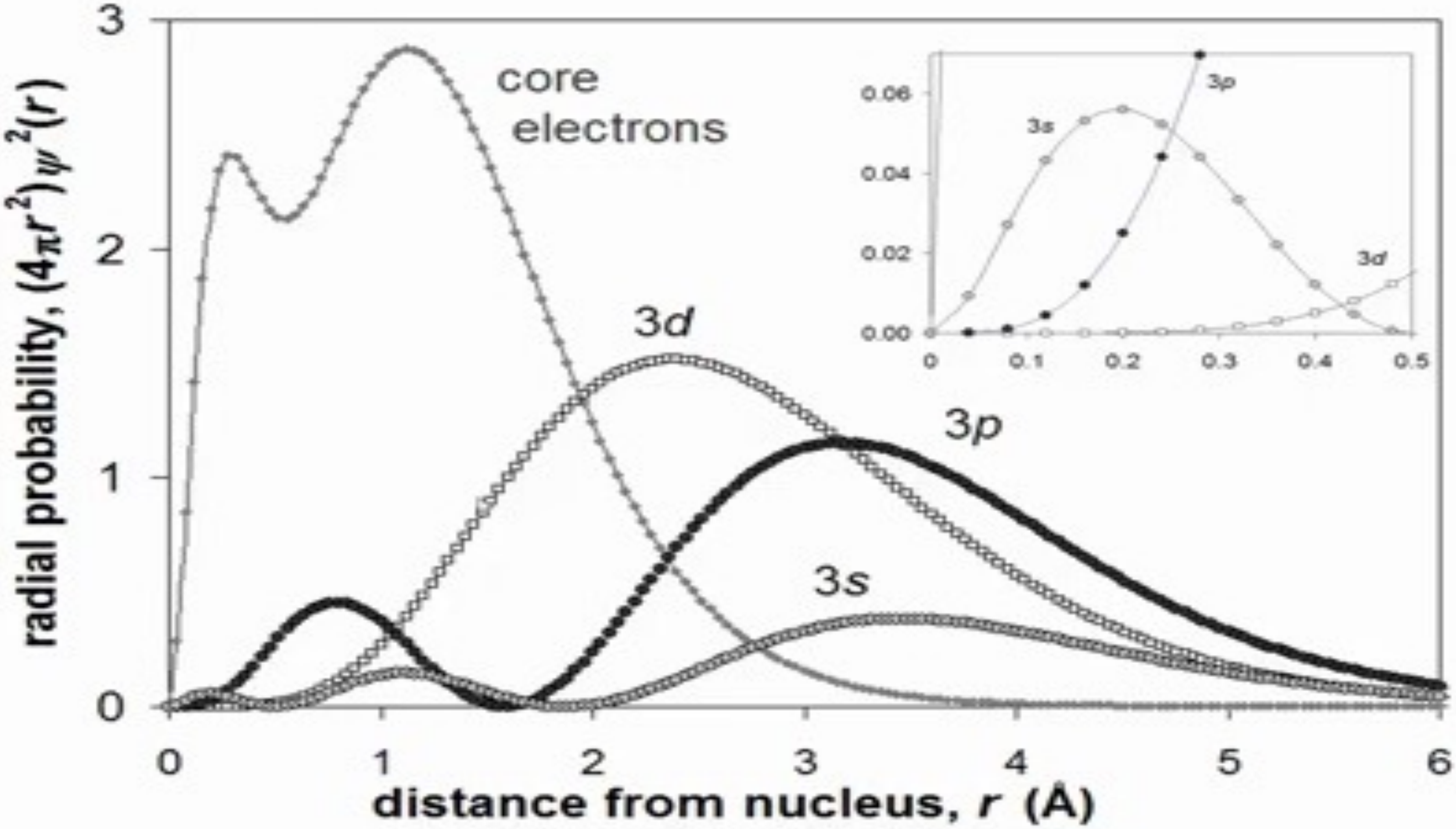
Periodic Table of Elements

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 H	Atomic # Symbol																2 He
2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
3	11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba	57–71	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra	89–103	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Uub	113 Uut	114 Uuq	115 Uup	116 Uuh	117 Uus	118 Uuo

For elements with no stable isotopes, the mass number of the isotope with the longest half-life is in parentheses.

57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

Azimuthal Quantum Number and Orbital Energy



Orbital Energies (in eV)

	H											**He**
1s	−13.5											−24.8
	Li	**Be**					**B**	**C**	**N**	**O**	**F**	**Ne**
2s	−5.3	−8.4					−13.4	−19.2	−26.0	−33.8	−42.6	−52.3
2p	---	---					−8.4	−11.0	−13.7	−16.6	−19.7	−23.0
	Na	**Mg**					**Al**	**Si**	**P**	**S**	**Cl**	**Ar**
3s	−4.9	−6.8					−10.7	−14.7	−19.2	−24.0	−29.1	−34.7
3p	---	---					−5.7	−7.5	−9.5	−11.5	−13.7	−16.0
	K	**Ca**	**Sc**	**Ti**		**Zn**	**Ga**	**Ge**	**As**	**Se**	**Br**	**Kr**
4s	−4.0	−5.3	−5.7	−6.0		−8.1	−11.7	−15.4	−19.2	−23.3	−27.6	−32.1
4p	---	---	---	---		---	−5.6	−7.3	−8.9	−10.6	−12.4	−14.3
3d	---	---	−9.1	−10.7		−20.6	−31.5	−43.4	−56.3	−70.3	−85.3	−101
	Rb	**Sr**	**Y**	**Zr**		**Cd**	**In**	**Sn**	**Sb**	**Te**	**I**	**Xe**
5s	−4.0	−4.9	−5.4	−5.8		−7.6	−10.7	−13.8	−16.9	−20.2	−23.7	−27.3
5p	---	---	---	---		---	−5.3	−6.7	−8.1	−9.6	−11.1	−12.6
4d	---	---	−6.3	−7.9		−19.5	−27.4	−35.5	−44.0	−53.0	−62.3	−72.2
	Cs	**Ba**	**La**	**Hf**		**Hg**	**Tl**	**Pb**	**Bi**	**Po**	**At**	**Rn**
6s	−3.5	−4.4	−4.9	−6.5		−8.9	−12.1	−15.3	−18.5	−21.9	−25.3	−28.9
6p	---	---	---	---		---	−5.2	−6.7	−8.1	−9.5	−11.0	−12.5
5d	---	---	−6.4	−6.5		−16.5	−23.0	−29.4	−35.9	−42.7	−49.6	−56.8

Orbital Energies (in eV)

	H										**He**
1s	–13.5										–24.8
	Li	**Be**				**B**	**C**	**N**	**O**	**F**	**Ne**
2s	–5.3	–8.4				–13.4	–19.2	–26.0	–33.8	–42.6	–52.3
2p	---	---				–8.4	–11.0	–13.7	–16.6	–19.7	–23.0
	Na	**Mg**				**Al**	**Si**	**P**	**S**	**Cl**	**Ar**
3s	–4.9	–6.8				–10.7	–14.7	–19.2	–24.0	–29.1	–34.7
3p	---	---				–5.7	–7.5	–9.5	–11.5	–13.7	–16.0
	K	**Ca**	**Sc**	**Ti**	**Zn**	**Ga**	**Ge**	**As**	**Se**	**Br**	**Kr**
4s	–4.0	–5.3	–5.7	–6.0	–8.1	–11.7	–15.4	–19.2	–23.3	–27.6	–32.1
4p	---	---	---	---	---	–5.6	–7.3	–8.9	–10.6	–12.4	–14.3
3d	---	---	–9.1	–10.7	–20.6	–31.5	–43.4	–56.3	–70.3	–85.3	–101
	Rb	**Sr**	**Y**	**Zr**	**Cd**	**In**	**Sn**	**Sb**	**Te**	**I**	**Xe**
5s	–4.0	–4.9	–5.4	–5.8	–7.6	–10.7	–13.8	–16.9	–20.2	–23.7	–27.3
5p	---	---	---	---	---	–5.3	–6.7	–8.1	–9.6	–11.1	–12.6
4d	---	---	–6.3	–7.9	–19.5	–27.4	–35.5	–44.0	–53.0	–62.3	–72.2
	Cs	**Ba**	**La**	**Hf**	**Hg**	**Tl**	**Pb**	**Bi**	**Po**	**At**	**Rn**
6s	–3.5	–4.4	–4.9	–6.5	–8.9	–12.1	–15.3	–18.5	–21.9	–25.3	–28.9
6p	---	---	---	---	---	–5.2	–6.7	–8.1	–9.5	–11.0	–12.5
5d	---	---	–6.4	–6.5	–16.5	–23.0	–29.4	–35.9	–42.7	–49.6	–56.8

Orbital Sizes

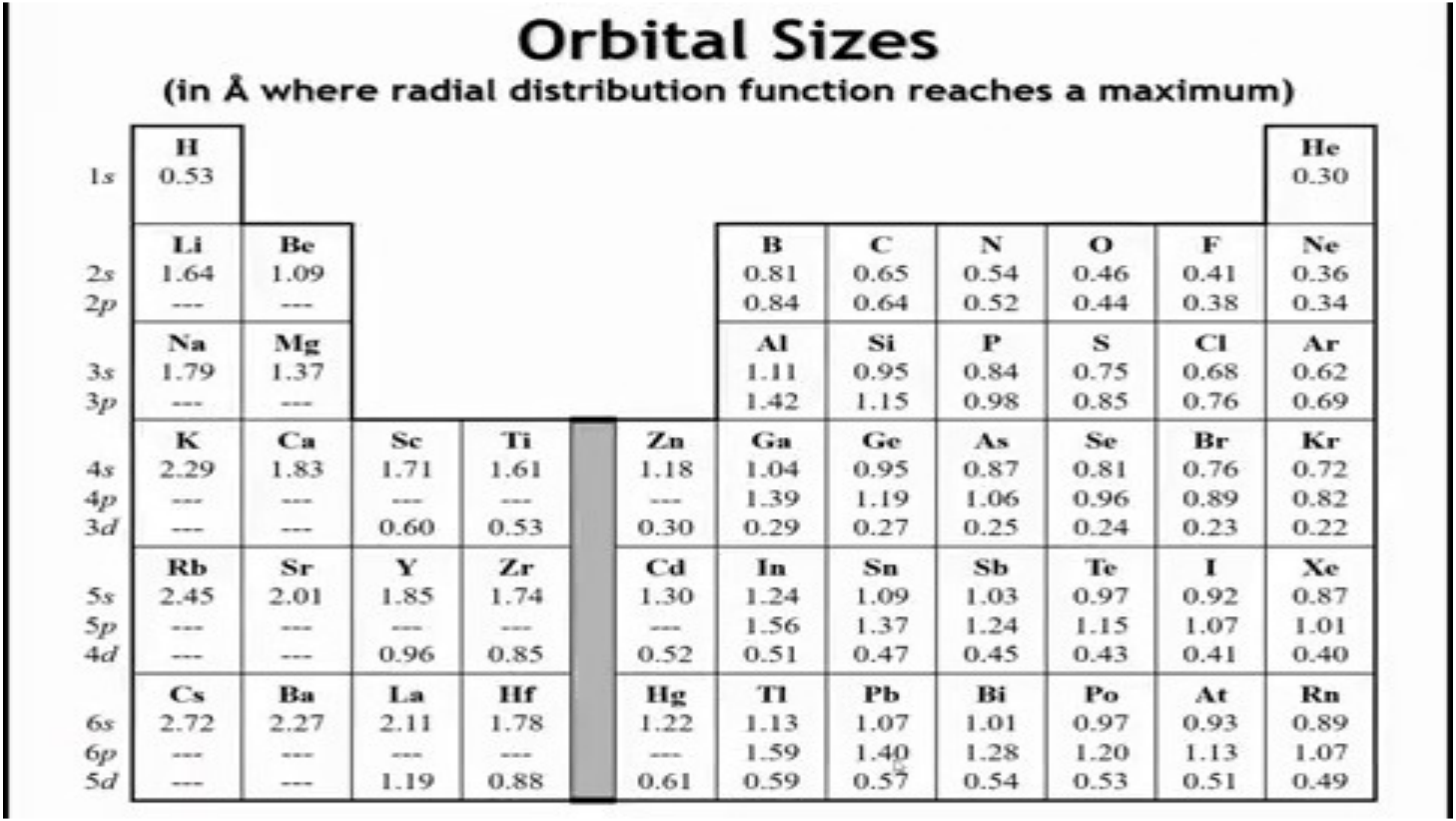
(in Å where radial distribution function reaches a maximum)

	H										**He**
1s	0.53										0.30
	Li	**Be**				**B**	**C**	**N**	**O**	**F**	**Ne**
2s	1.64	1.09				0.81	0.65	0.54	0.46	0.41	0.36
2p	---	---				0.84	0.64	0.52	0.44	0.38	0.34
	Na	**Mg**				**Al**	**Si**	**P**	**S**	**Cl**	**Ar**
3s	1.79	1.37				1.11	0.95	0.84	0.75	0.68	0.62
3p	---	---				1.42	1.15	0.98	0.85	0.76	0.69
	K	**Ca**	**Sc**	**Ti**	**Zn**	**Ga**	**Ge**	**As**	**Se**	**Br**	**Kr**
4s	2.29	1.83	1.71	1.61	1.18	1.04	0.95	0.87	0.81	0.76	0.72
4p	---	---	---	---	---	1.39	1.19	1.06	0.96	0.89	0.82
3d	---	---	0.60	0.53	0.30	0.29	0.27	0.25	0.24	0.23	0.22
	Rb	**Sr**	**Y**	**Zr**	**Cd**	**In**	**Sn**	**Sb**	**Te**	**I**	**Xe**
5s	2.45	2.01	1.85	1.74	1.30	1.24	1.09	1.03	0.97	0.92	0.87
5p	---	---	---	---	---	1.56	1.37	1.24	1.15	1.07	1.01
4d	---	---	0.96	0.85	0.52	0.51	0.47	0.45	0.43	0.41	0.40
	Cs	**Ba**	**La**	**Hf**	**Hg**	**Tl**	**Pb**	**Bi**	**Po**	**At**	**Rn**
6s	2.72	2.27	2.11	1.78	1.22	1.13	1.07	1.01	0.97	0.93	0.89
6p	---	---	---	---	---	1.59	1.40	1.28	1.20	1.13	1.07
5d	---	---	1.19	0.88	0.61	0.59	0.57	0.54	0.53	0.51	0.49

Orbital Sizes

(in Å where radial distribution function reaches a maximum)

	H											**He**
1*s*	0.53											0.30
	Li	**Be**					**B**	**C**	**N**	**O**	**F**	**Ne**
2*s*	1.64	1.09					0.81	0.65	0.54	0.46	0.41	0.36
2*p*	---	---					0.84	0.64	0.52	0.44	0.38	0.34
	Na	**Mg**					**Al**	**Si**	**P**	**S**	**Cl**	**Ar**
3*s*	1.79	1.37					1.11	0.95	0.84	0.75	0.68	0.62
3*p*	---	---					1.42	1.15	0.98	0.85	0.76	0.69
	K	**Ca**	**Sc**	**Ti**		**Zn**	**Ga**	**Ge**	**As**	**Se**	**Br**	**Kr**
4*s*	2.29	1.83	1.71	1.61		1.18	1.04	0.95	0.87	0.81	0.76	0.72
4*p*	---	---	---	---		---	1.39	1.19	1.06	0.96	0.89	0.82
3*d*	---	---	0.60	0.53		0.30	0.29	0.27	0.25	0.24	0.23	0.22
	Rb	**Sr**	**Y**	**Zr**		**Cd**	**In**	**Sn**	**Sb**	**Te**	**I**	**Xe**
5*s*	2.45	2.01	1.85	1.74		1.30	1.24	1.09	1.03	0.97	0.92	0.87
5*p*	---	---	---	---		---	1.56	1.37	1.24	1.15	1.07	1.01
4*d*	---	---	0.96	0.85		0.52	0.51	0.47	0.45	0.43	0.41	0.40
	Cs	**Ba**	**La**	**Hf**		**Hg**	**Tl**	**Pb**	**Bi**	**Po**	**At**	**Rn**
6*s*	2.72	2.27	2.11	1.78		1.22	1.13	1.07	1.01	0.97	0.93	0.89
6*p*	---	---	---	---		---	1.59	1.40	1.28	1.20	1.13	1.07
5*d*	---	---	1.19	0.88		0.61	0.59	0.57	0.54	0.53	0.51	0.49



Orbital Sizes

(in Å where radial distribution function reaches a maximum)

	H										**He**
1*s*	0.53										0.30
	Li	**Be**				**B**	**C**	**N**	**O**	**F**	**Ne**
2*s*	1.64	1.09				0.81	0.65	0.54	0.46	0.41	0.36
2*p*	---	---				0.84	0.64	0.52	0.44	0.38	0.34
	Na	**Mg**				**Al**	**Si**	**P**	**S**	**Cl**	**Ar**
3*s*	1.79	1.37				1.11	0.95	0.84	0.75	0.68	0.62
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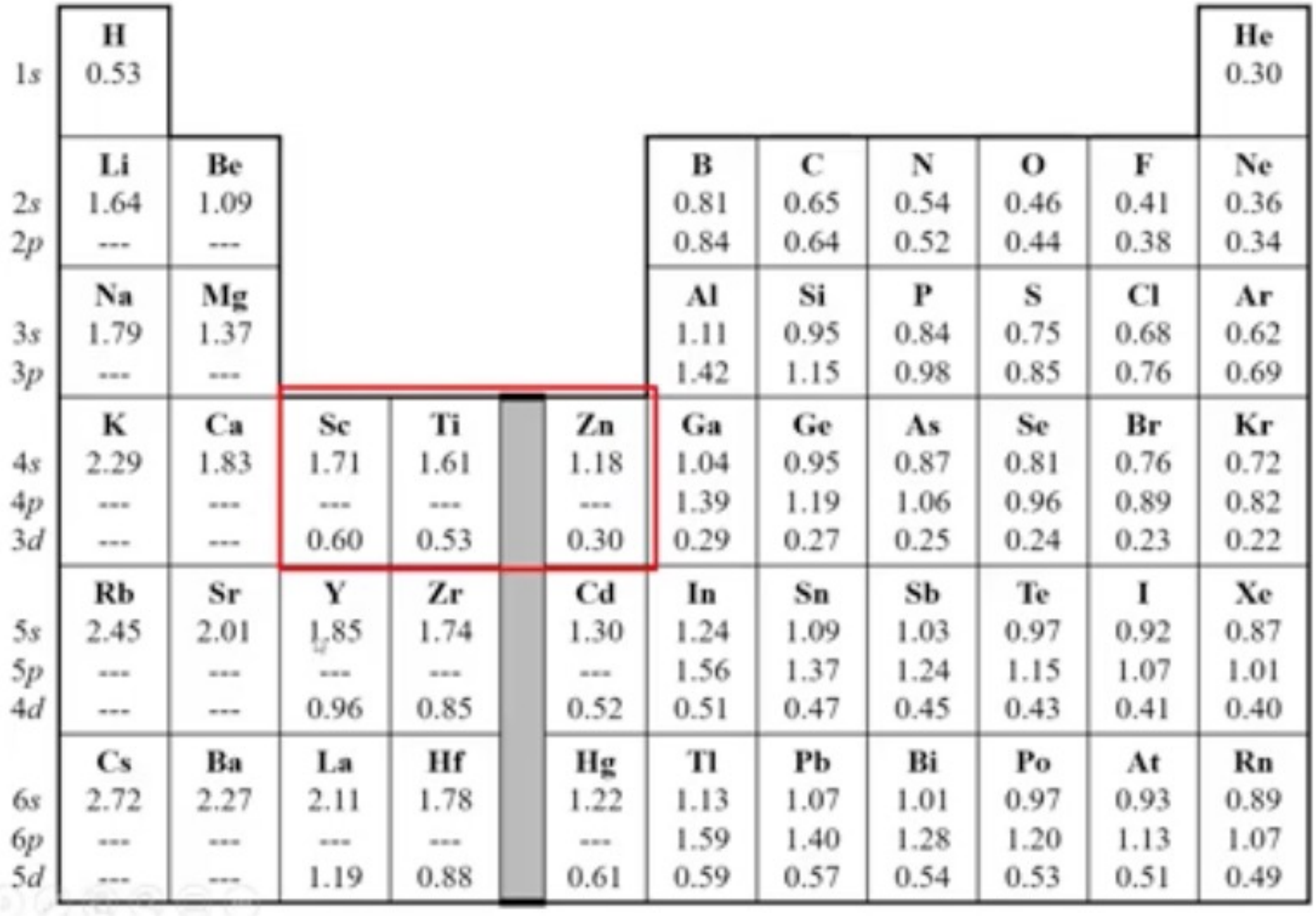
	K	**Ca**	**Sc**	**Ti**	**Zn**	**Ga**	**Ge**	**As**	**Se**	**Br**	**Kr**
4*s*	2.29	1.83	1.71	1.61	1.18	1.04	0.95	0.87	0.81	0.76	0.72
4*p*	---	---	---	---	---	1.39	1.19	1.06	0.96	0.89	0.82
3*d*	---	---	0.60	0.53	0.30	0.29	0.27	0.25	0.24	0.23	0.22
	Rb	**Sr**	**Y**	**Zr**	**Cd**	**In**	**Sn**	**Sb**	**Te**	**I**	**Xe**
5*s*	2.45	2.01	1.85	1.74	1.30	1.24	1.09	1.03	0.97	0.92	0.87
5*p*	---	---	---	---	---	1.56	1.37	1.24	1.15	1.07	1.01
4*d*	---	---	0.96	0.85	0.52	0.51	0.47	0.45	0.43	0.41	0.40
	Cs	**Ba**	**La**	**Hf**	**Hg**	**Tl**	**Pb**	**Bi**	**Po**	**At**	**Rn**
6*s*	2.72	2.27	2.11	1.78	1.22	1.13	1.07	1.01	0.97	0.93	0.89
6*p*	---	---	---	---	---	1.59	1.40	1.28	1.20	1.13	1.07
5*d*	---	---	1.19	0.88	0.61	0.59	0.57	0.54	0.53	0.51	0.49

Orbital Sizes

(in Å where radial distribution function reaches a maximum)



	H											**He**
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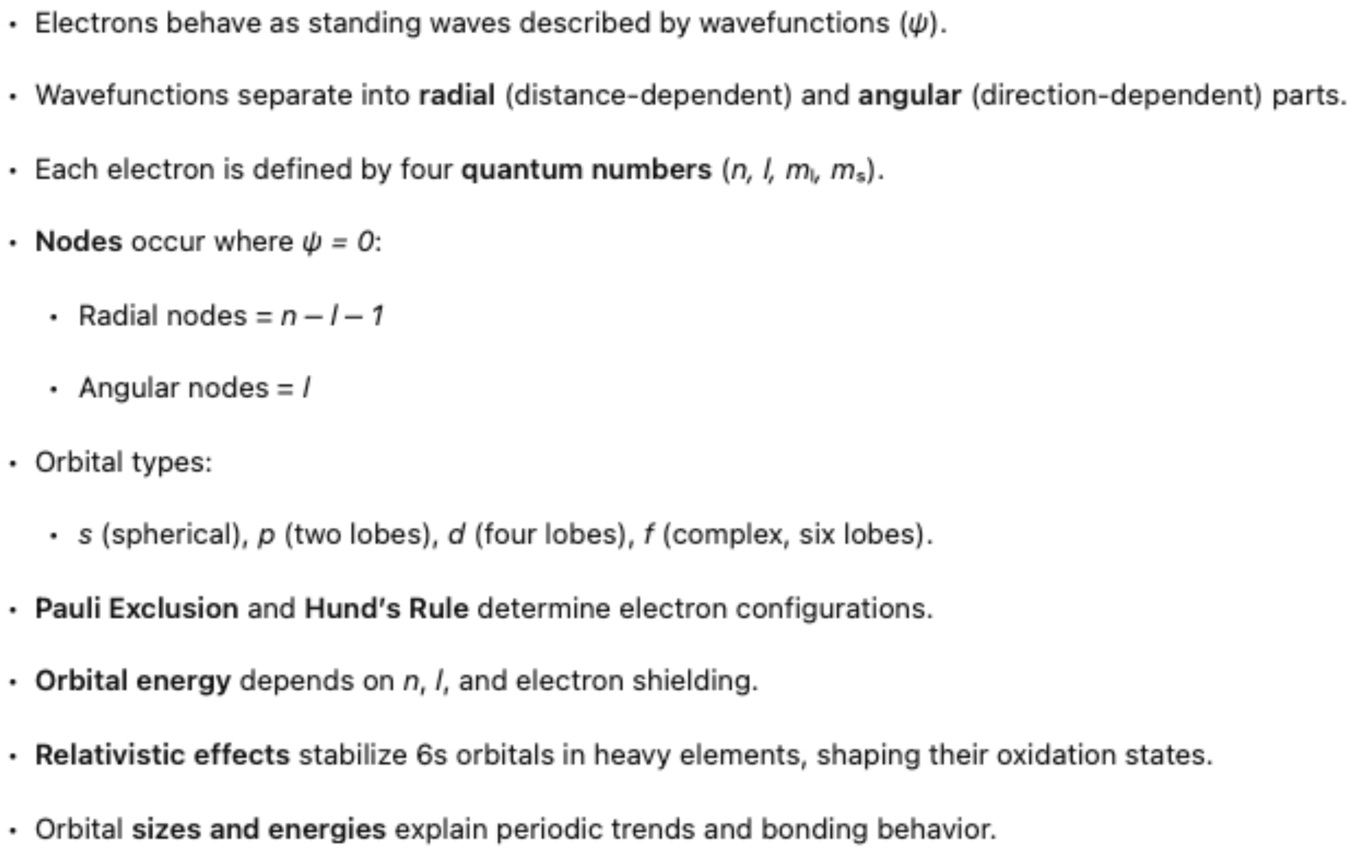
	Li	**Be**					**B**	**C**	**N**	**O**	**F**	**Ne**
2*s*	1.64	1.09					0.81	0.65	0.54	0.46	0.41	0.36
2*p*	---	---					0.84	0.64	0.52	0.44	0.38	0.34
	Na	**Mg**					**Al**	**Si**	**P**	**S**	**Cl**	**Ar**
3*s*	1.79	1.37					1.11	0.95	0.84	0.75	0.68	0.62
3*p*	---	---					1.42	1.15	0.98	0.85	0.76	0.69
	K	**Ca**	**Sc**	**Ti**		**Zn**	**Ga**	**Ge**	**As**	**Se**	**Br**	**Kr**
4*s*	2.29	1.83	1.71	1.61		1.18	1.04	0.95	0.87	0.81	0.76	0.72
4*p*	---	---	---	---		---	1.39	1.19	1.06	0.96	0.89	0.82
3*d*	---	---	0.60	0.53		0.30	0.29	0.27	0.25	0.24	0.23	0.22
	Rb	**Sr**	**Y**	**Zr**		**Cd**	**In**	**Sn**	**Sb**	**Te**	**I**	**Xe**
5*s*	2.45	2.01	1.85	1.74		1.30	1.24	1.09	1.03	0.97	0.92	0.87
5*p*	---	---	---	---		---	1.56	1.37	1.24	1.15	1.07	1.01
4*d*	---	---	0.96	0.85		0.52	0.51	0.47	0.45	0.43	0.41	0.40
	Cs	**Ba**	**La**	**Hf**		**Hg**	**Tl**	**Pb**	**Bi**	**Po**	**At**	**Rn**
6*s*	2.72	2.27	2.11	1.78		1.22	1.13	1.07	1.01	0.97	0.93	0.89
6*p*	---	---	---	---		---	1.59	1.40	1.28	1.20	1.13	1.07
5*d*	---	---	1.19	0.88		0.61	0.59	0.57	0.54	0.53	0.51	0.49

Summary



- Electrons behave as standing waves described by wavefunctions (ψ).
- Wavefunctions separate into **radial** (distance-dependent) and **angular** (direction-dependent) parts.
- Each electron is defined by four **quantum numbers** (n, l, m_l, m_s).
- **Nodes** occur where $\psi = 0$:
  - Radial nodes = $n - l - 1$
  - Angular nodes = l
- Orbital types:
  - *s* (spherical), *p* (two lobes), *d* (four lobes), *f* (complex, six lobes).
- **Pauli Exclusion** and **Hund's Rule** determine electron configurations.
- **Orbital energy** depends on n, l, and electron shielding.
- **Relativistic effects** stabilize 6s orbitals in heavy elements, shaping their oxidation states.
- Orbital **sizes and energies** explain periodic trends and bonding behavior.

1. How does the number of radial and angular nodes in an orbital relate to the quantum numbers, and why is this relationship significant for understanding bonding in solids?

1. How does the number of radial and angular nodes in an orbital relate to the quantum numbers, and why is this relationship significant for understanding bonding in solids?

The number of **radial nodes** equals $n - l - 1$, and the number of **angular (nodal planes)** equals l. For example, a 3s orbital ($n = 3$, $l = 0$) has two radial nodes, while a 3d orbital ($n = 3$, $l = 2$) has two angular nodes. This relationship is significant because the presence and type of nodes determine orbital shapes and electron density distribution, which in turn control orbital overlap and bonding directionality in solids

2. Why are 3d orbitals higher in energy than 4s orbitals in potassium but lower in energy by the time we reach zinc, and how does this trend affect the chemistry of transition metals?

2. Why are 3d orbitals higher in energy than 4s orbitals in potassium but lower in energy by the time we reach zinc, and how does this trend affect the chemistry of transition metals?

In early transition metals (e.g., K, Ca), 4s orbitals lie lower in energy because they penetrate closer to the nucleus. As we add more d electrons, electron–electron repulsion and poor shielding by d orbitals lower the 3d energies until they become core-like by zinc. Consequently, transition metals preferentially lose 4s rather than 3d electrons during oxidation, explaining the stable +2 oxidation state of zinc and the variability of oxidation states across the transition series

3. What causes the “inert pair effect” observed in heavy p-block elements, and how does this arise from relativistic effects?

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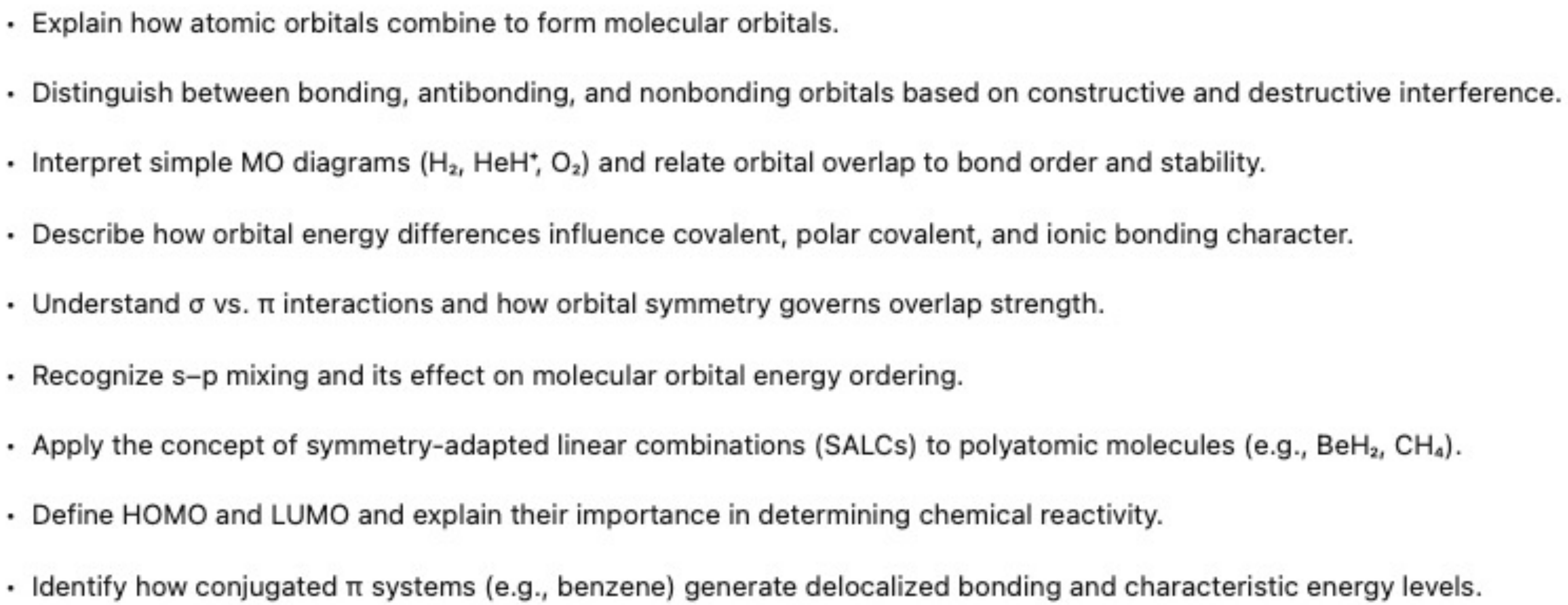
In heavy atoms like thallium and lead, the **6s orbitals** are relativistically stabilized because inner electrons move at speeds approaching light, increasing their effective mass and contraction. This lowers the energy of s orbitals relative to p orbitals by 2–3 eV more than expected, reducing the tendency of the s electrons to participate in bonding. The result is stabilization of lower oxidation states such as Pb^{2+} over Pb^{4+}

4. Why do second-period elements (C, N, O) form strong π bonds, whereas heavier congeners (Si, P, S) rarely do, and what orbital property explains this difference?

4. Why do second-period elements (C, N, O) form strong π bonds, whereas heavier congeners (Si, P, S) rarely do, and what orbital property explains this difference?

The 2p orbitals of second-period elements are **anomalously small and similar in size to 2s orbitals**, enabling effective side-by-side overlap for π bonding. In contrast, 3p orbitals in heavier elements are much larger and diffuse, leading to poor overlap and weak π bonding. This size similarity between 2s and 2p orbitals underlies the rich π-bond chemistry of carbon and its importance in organic and solid-state structures

Molecular Orbital Theory



- Explain how atomic orbitals combine to form molecular orbitals.
- Distinguish between bonding, antibonding, and nonbonding orbitals based on constructive and destructive interference.
- Interpret simple MO diagrams (H_2, HeH^+, O_2) and relate orbital overlap to bond order and stability.
- Describe how orbital energy differences influence covalent, polar covalent, and ionic bonding character.
- Understand σ vs. π interactions and how orbital symmetry governs overlap strength.
- Recognize s–p mixing and its effect on molecular orbital energy ordering.
- Apply the concept of symmetry-adapted linear combinations (SALCs) to polyatomic molecules (e.g., BeH_2, CH_4).
- Define HOMO and LUMO and explain their importance in determining chemical reactivity.
- Identify how conjugated π systems (e.g., benzene) generate delocalized bonding and characteristic energy levels.

Molecular Orbitals

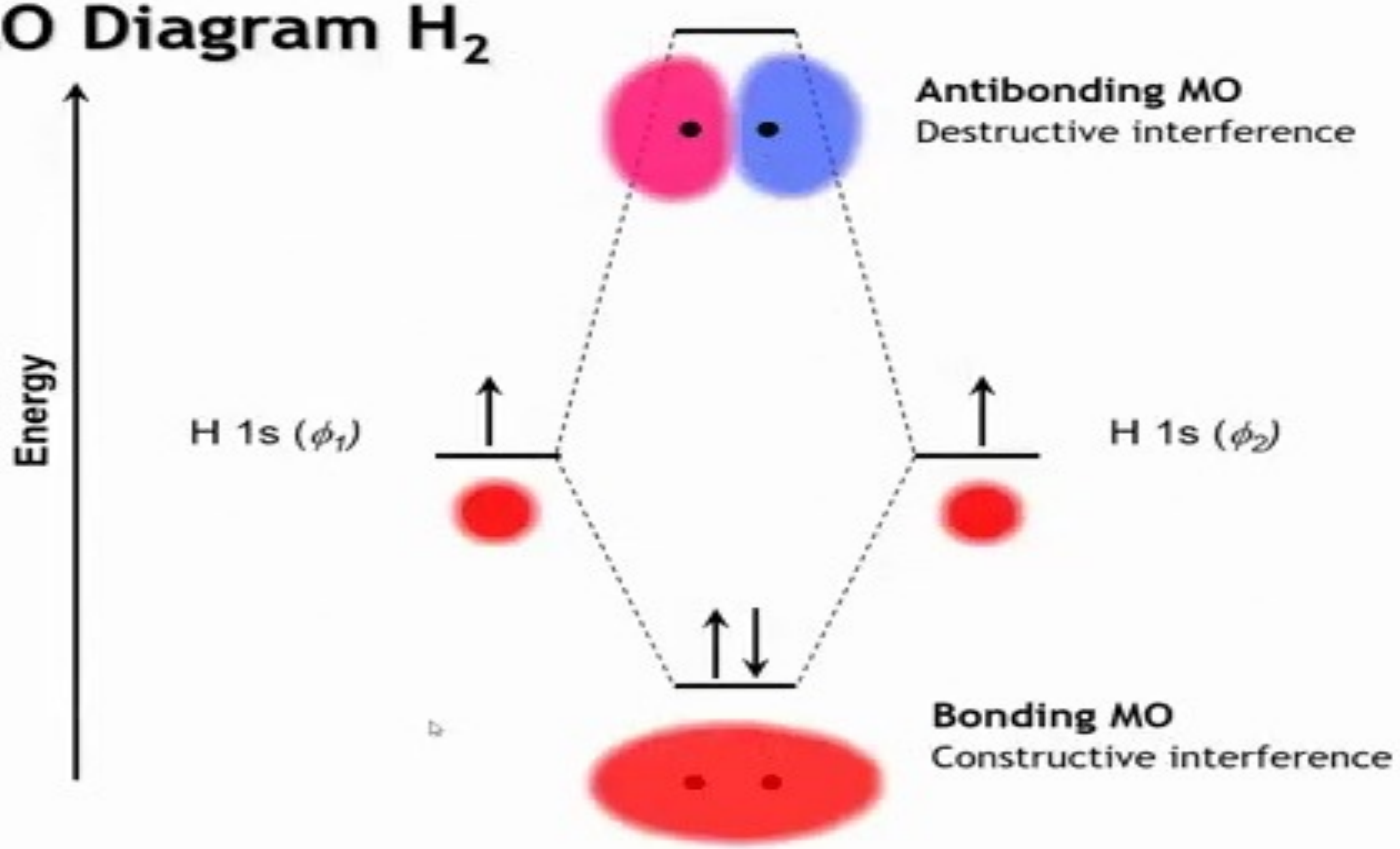
The electrons in an atom reside in atomic orbitals, each of which has a characteristic wavefunction.

When atoms combine to form molecules we need new orbitals, **molecular orbitals**, that have their own wavefunctions.

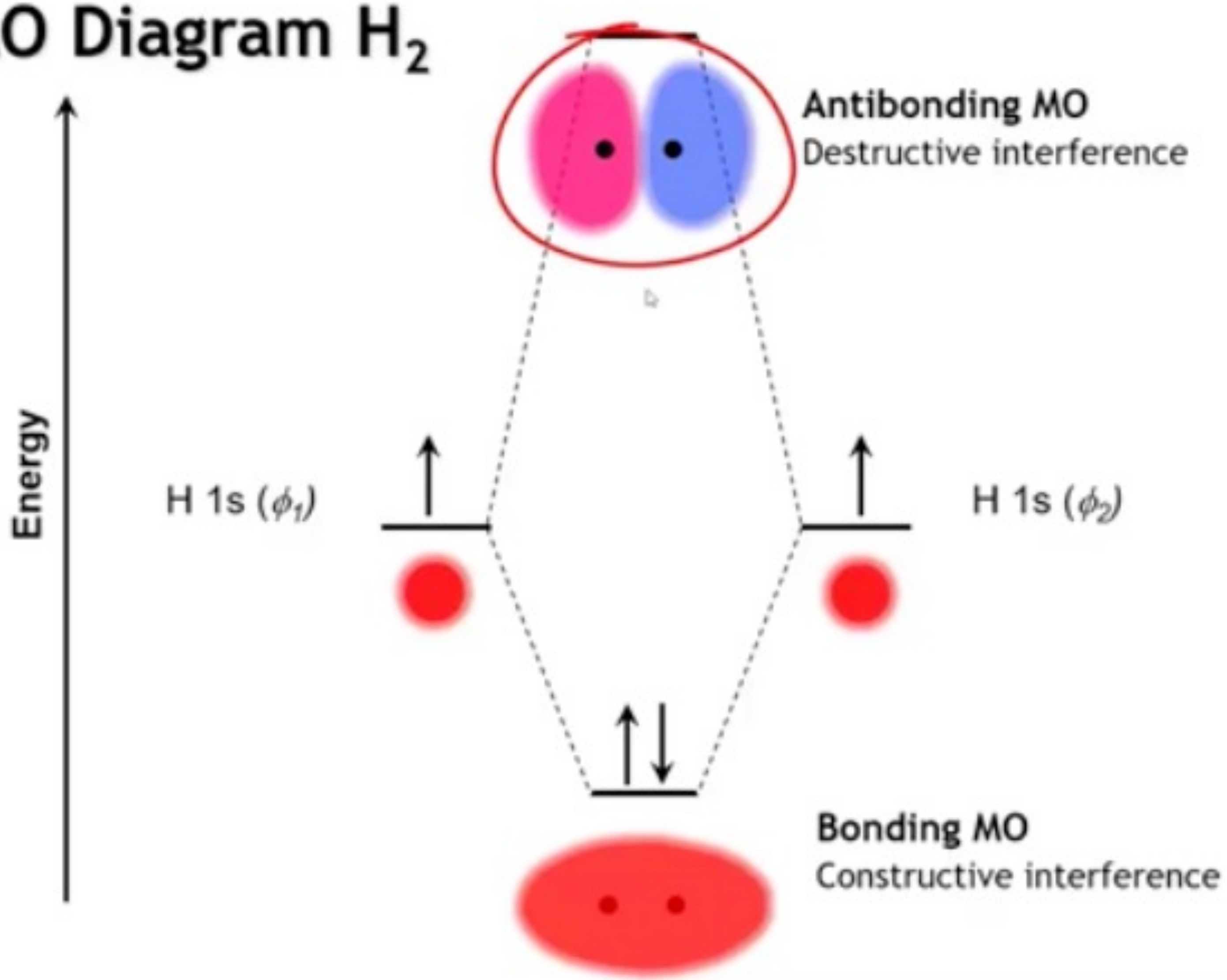
We will choose to describe molecular orbital wavefunctions as linear combination of atomic orbital wavefunctions (LCAO):

$$\psi_{MO} = \sum c_1\psi_{AO(1)} + c_2\psi_{AO(2)} + \ \ldots c_i\psi_{AO(i)}$$

MO Diagram H_2



MO Diagram H_2



Energy

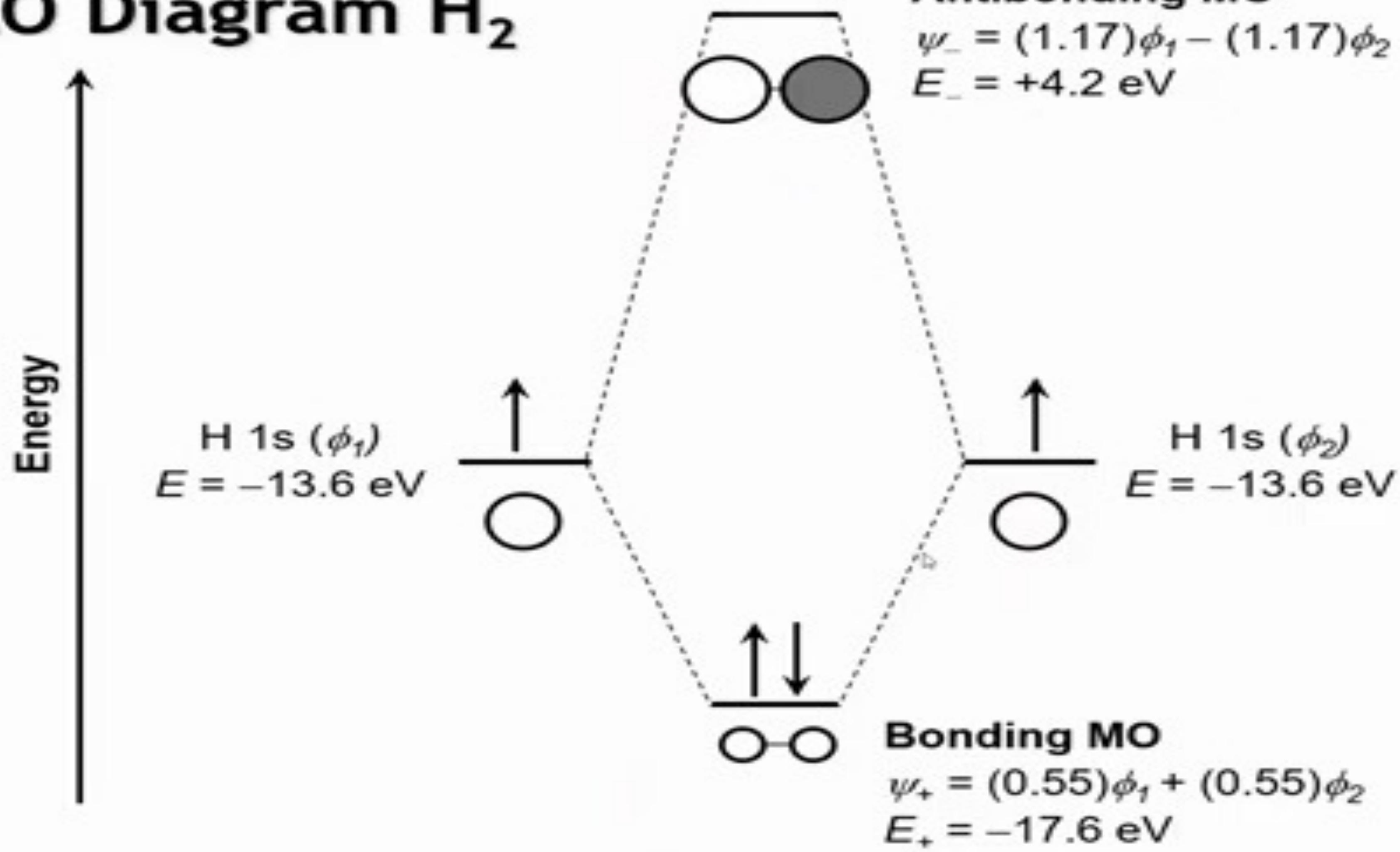
Antibonding MO
Destructive interference

H 1s (ϕ_1)

H 1s (ϕ_2)

Bonding MO
Constructive interference

MO Diagram H_2



Antibonding MO

$\psi_{-} = (1.17)\phi_1 - (1.17)\phi_2$

$E_{-} = +4.2$ eV

H 1s (ϕ_1)

$E = -13.6$ eV

H 1s (ϕ_2)

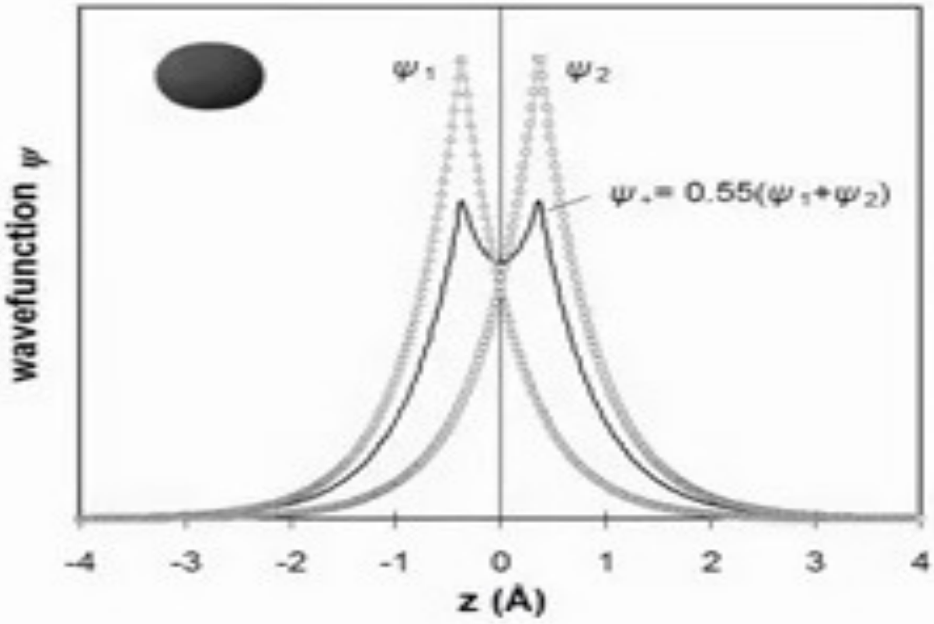
$E = -13.6$ eV

Bonding MO

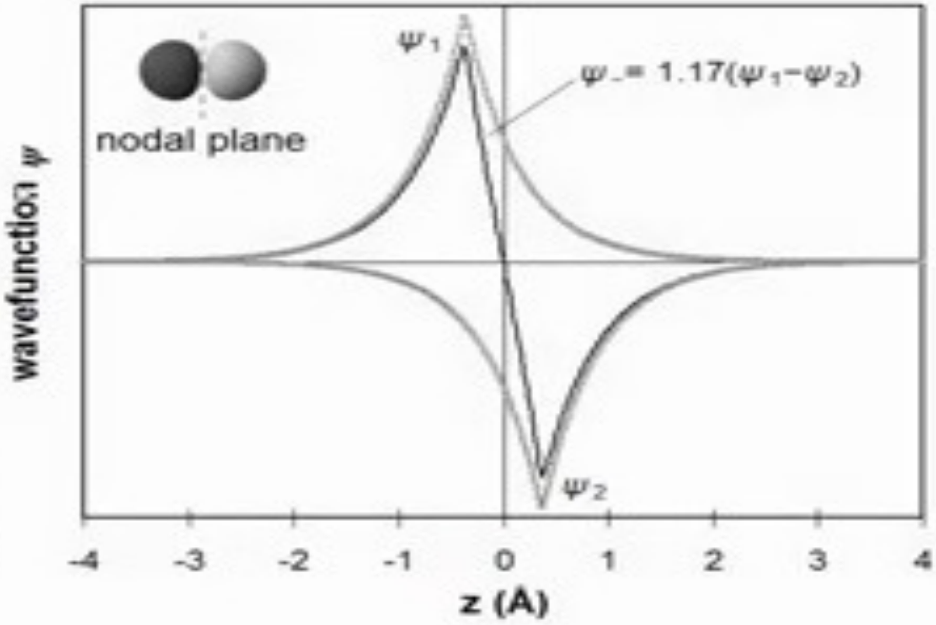
$\psi_{+} = (0.55)\phi_1 + (0.55)\phi_2$

$E_{+} = -17.6$ eV

Molecular Orbital Wavefunctions

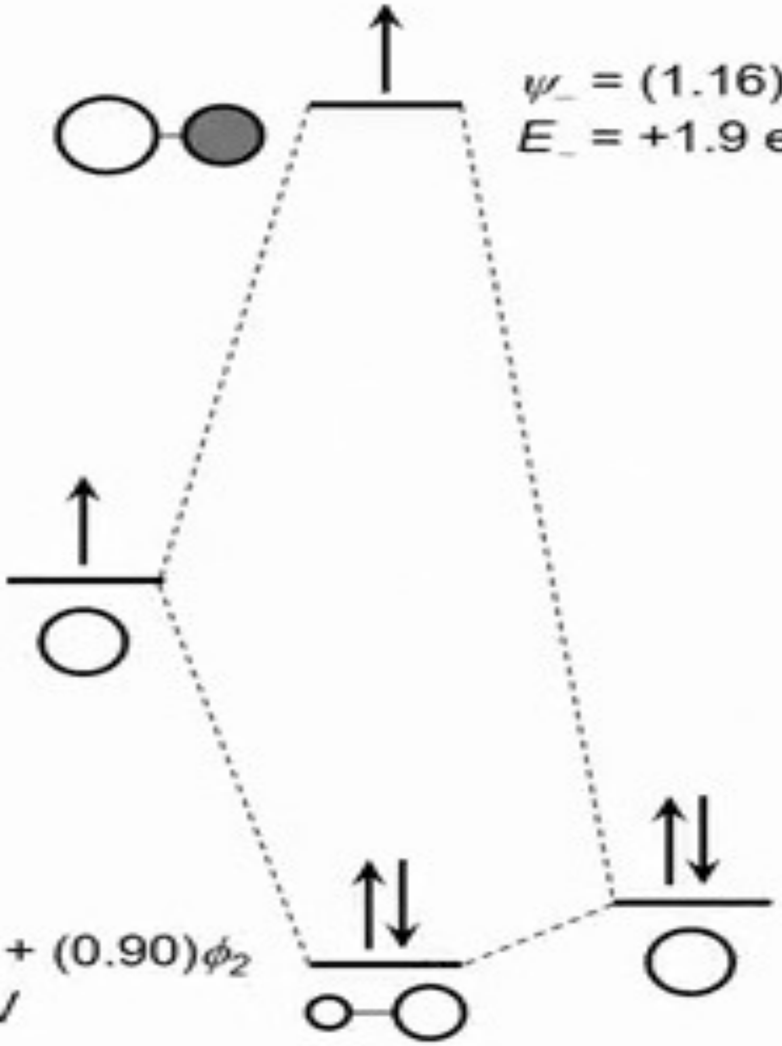


Bonding MO
- Constructive interference
- Increases e^- between nuclei
- Lower energy



Antibonding MO
- Destructive interference
- Nodal plane between nuclei
- Higher energy

HHe



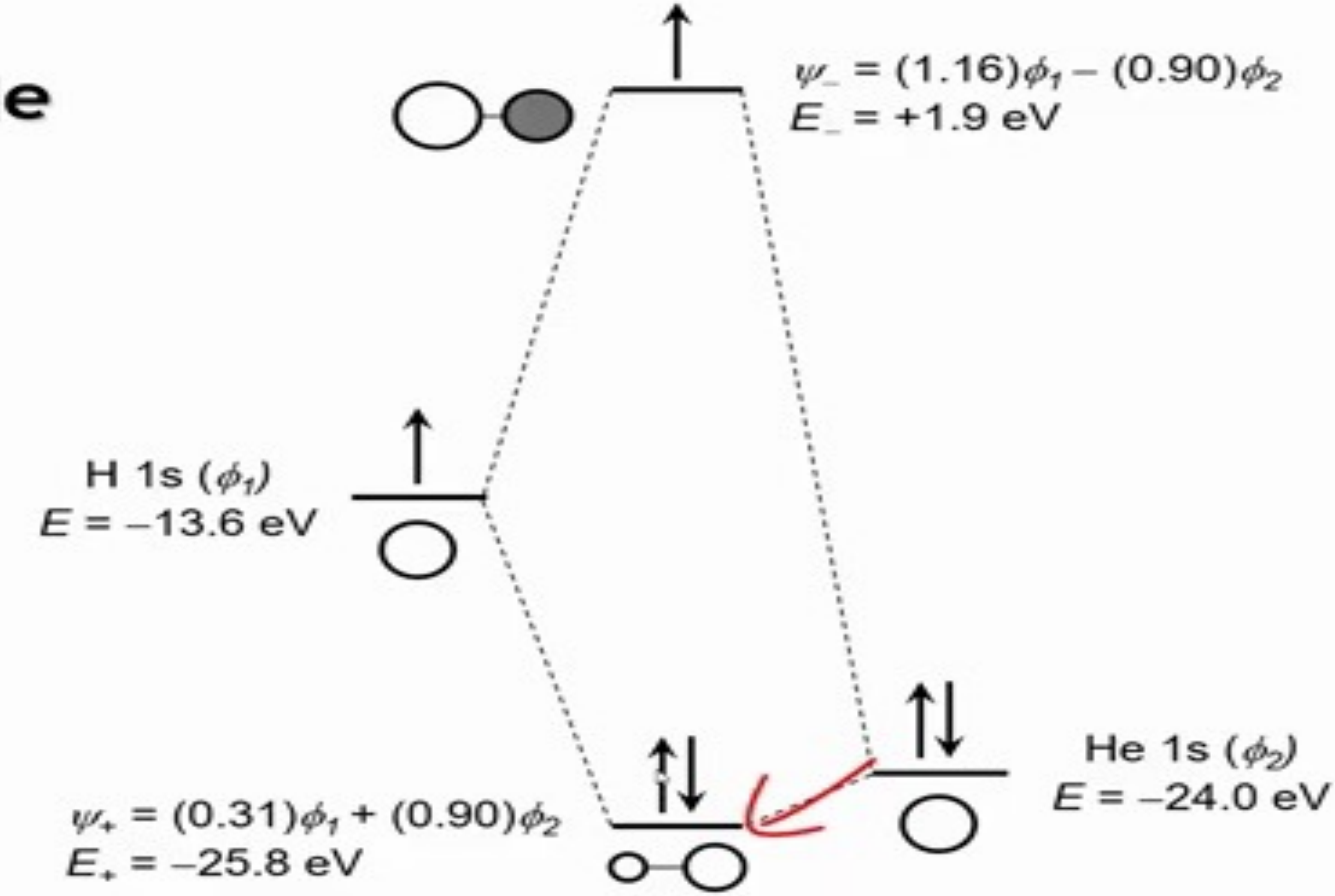
$\psi_- = (1.16)\phi_1 - (0.90)\phi_2$
$E_- = +1.9$ eV

H 1s (ϕ_1)
$E = -13.6$ eV

He 1s (ϕ_2)
$E = -24.0$ eV

$\psi_+ = (0.31)\phi_1 + (0.90)\phi_2$
$E_+ = -25.8$ eV

HHe



$\psi_{-} = (1.16)\phi_1 - (0.90)\phi_2$

$E_{-} = +1.9$ eV

H 1s (ϕ_1)

$E = -13.6$ eV

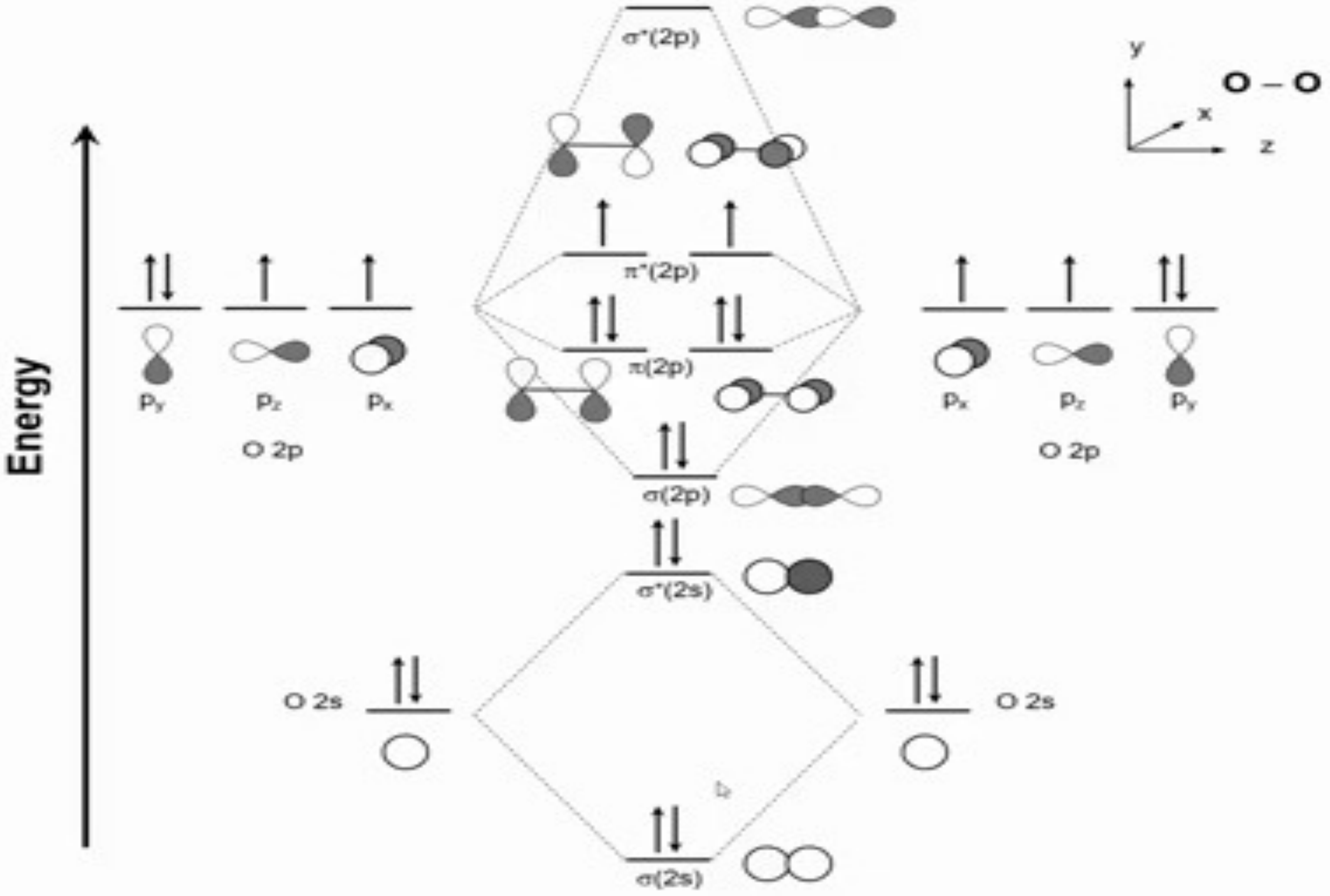
He 1s (ϕ_2)

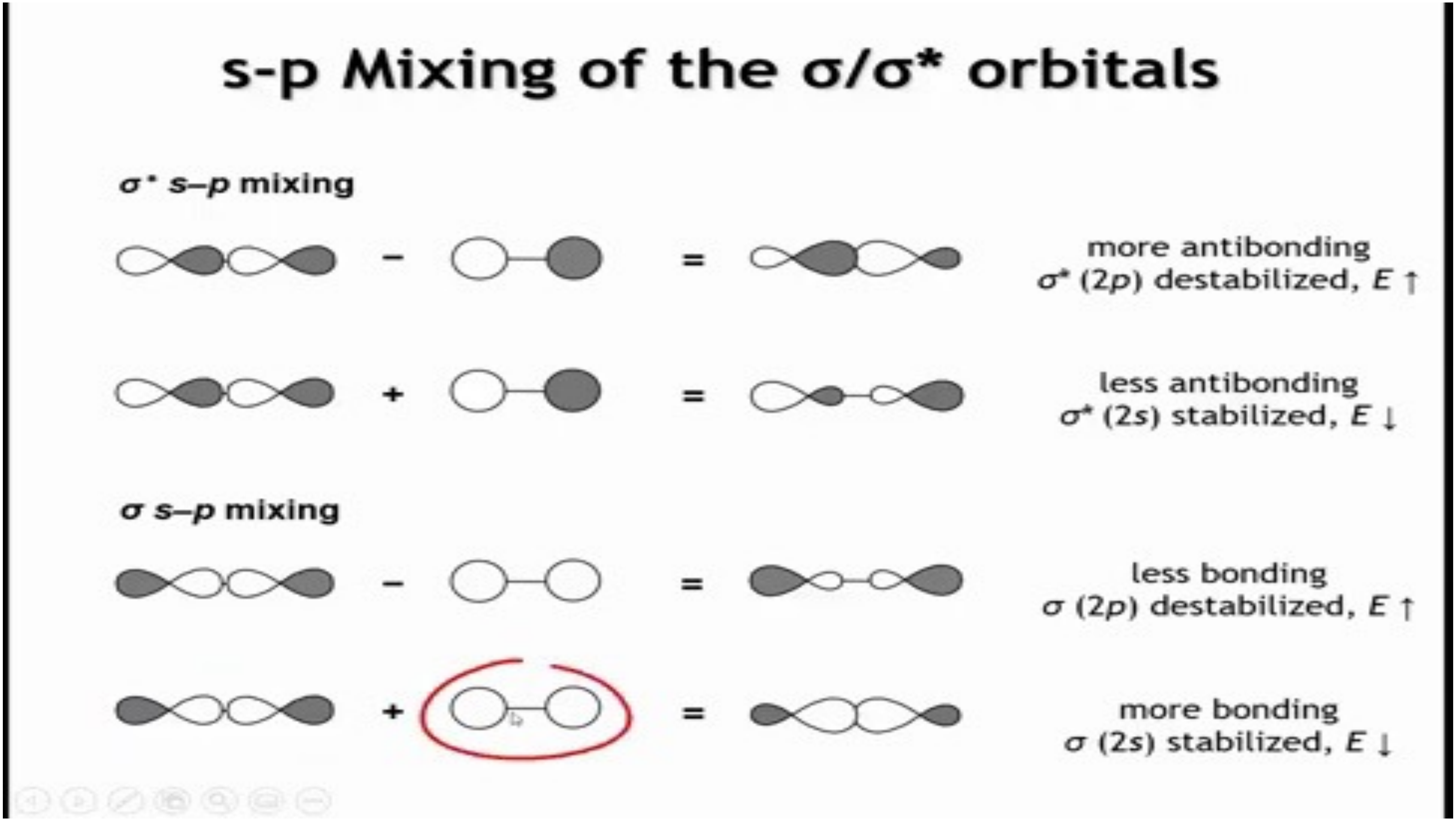
$E = -24.0$ eV

$\psi_{+} = (0.31)\phi_1 + (0.90)\phi_2$

$E_{+} = -25.8$ eV

O_2


σ*(2p)
y
x
z
O – O
π*(2p)
π(2p)
Energy
p_y
p_z
p_x
O 2p
p_x
p_z
p_y
O 2p
σ(2p)
σ*(2s)
O 2s
O 2s
σ(2s)



s-p Mixing of the σ/σ* orbitals

σ^* *s–p* mixing

more antibonding
σ^* (2p) destabilized, E ↑

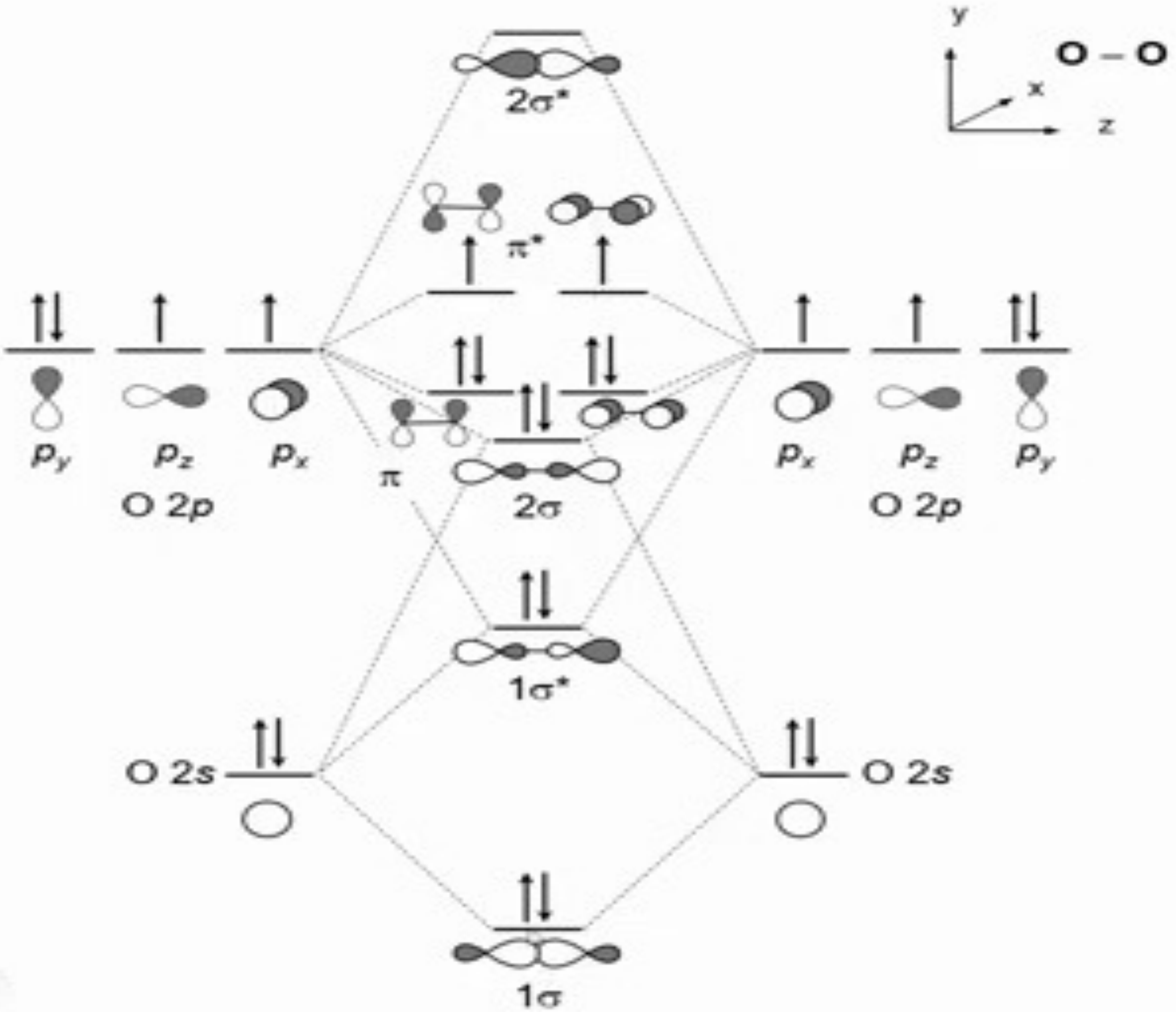
less antibonding
σ^* (2s) stabilized, E ↓

σ *s–p* mixing

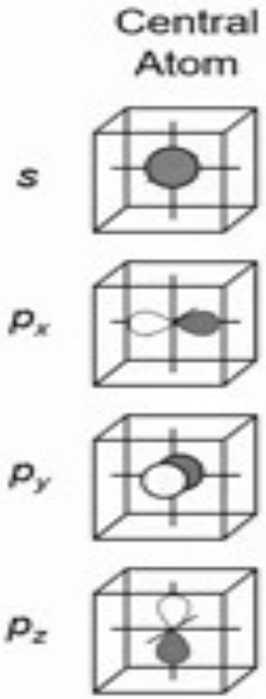
less bonding
σ (2p) destabilized, E ↑

more bonding
σ (2s) stabilized, E ↓

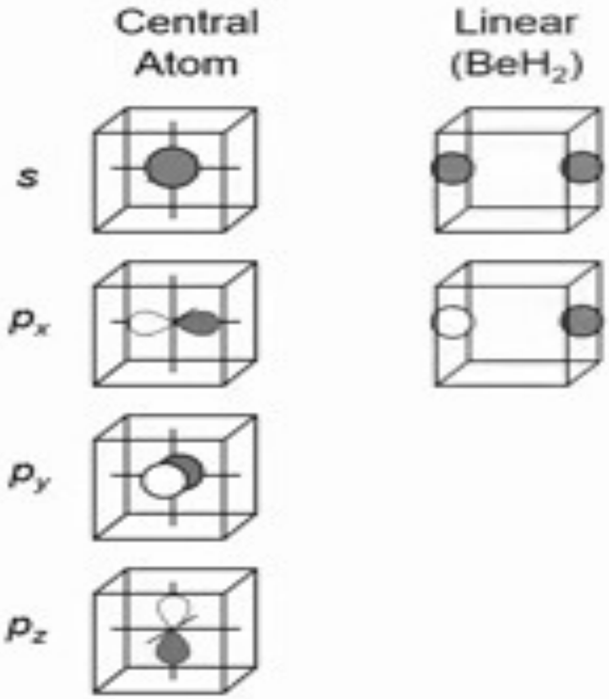
O_2



Beyond diatomics

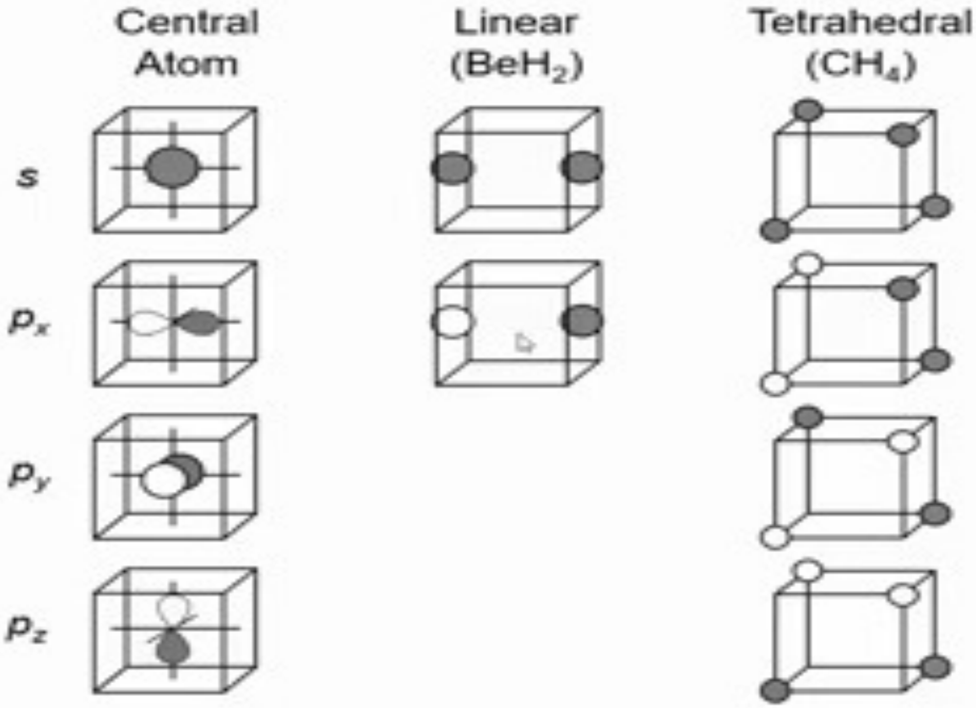


Beyond diatomics



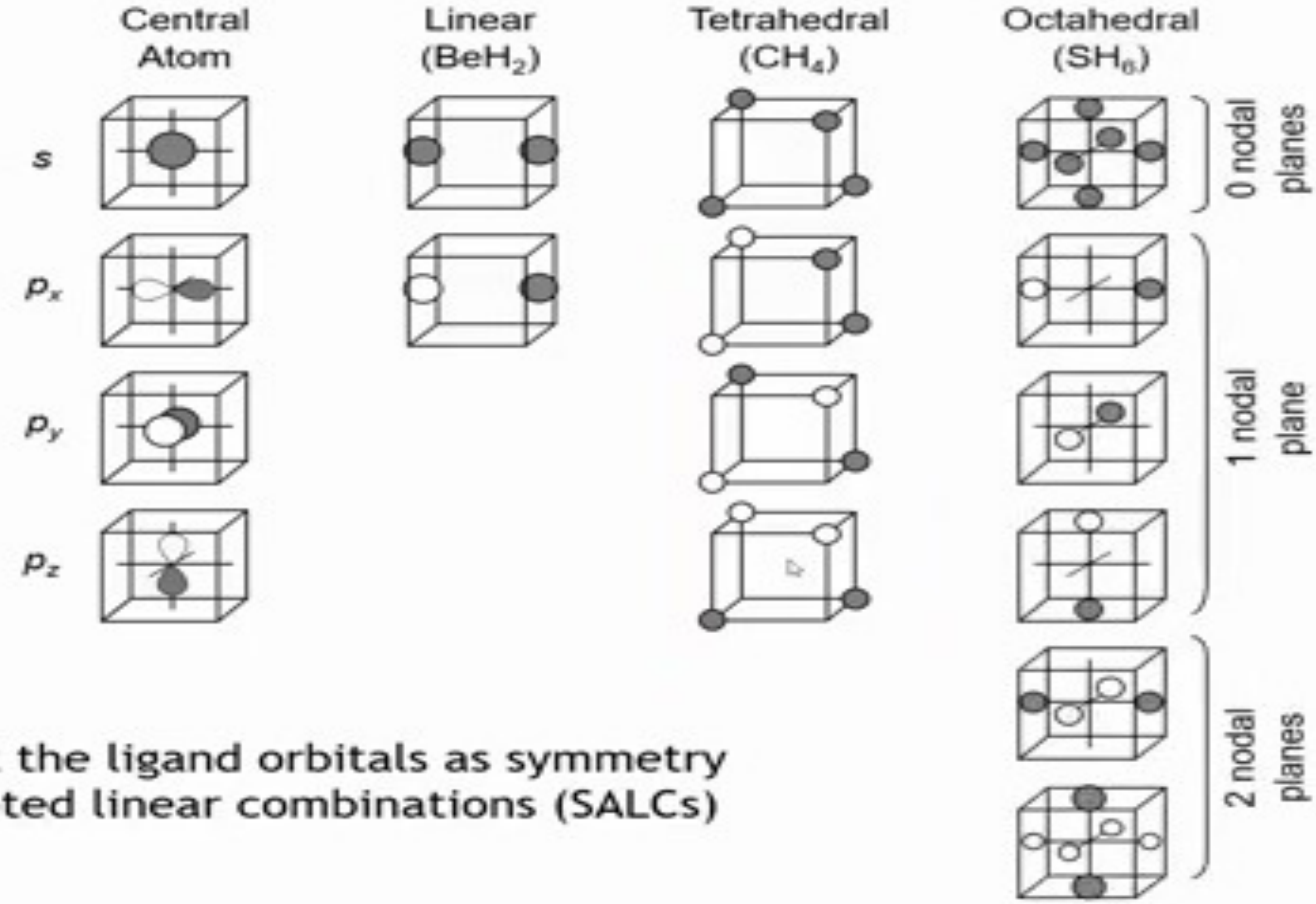
Treat the ligand orbitals as symmetry adapted linear combinations (SALCs)

Beyond diatomics



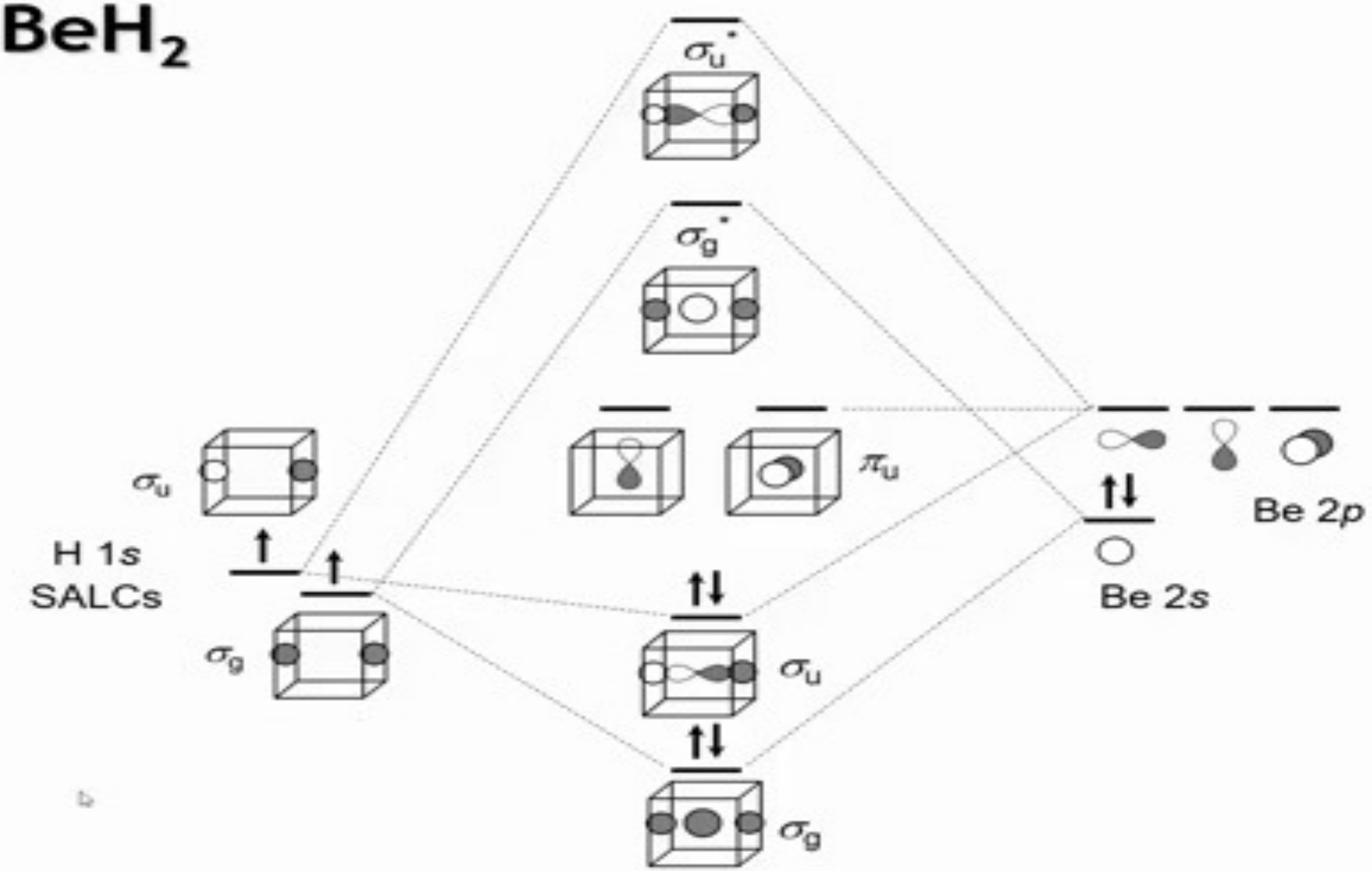
Treat the ligand orbitals as symmetry adapted linear combinations (SALCs)

Beyond diatomics

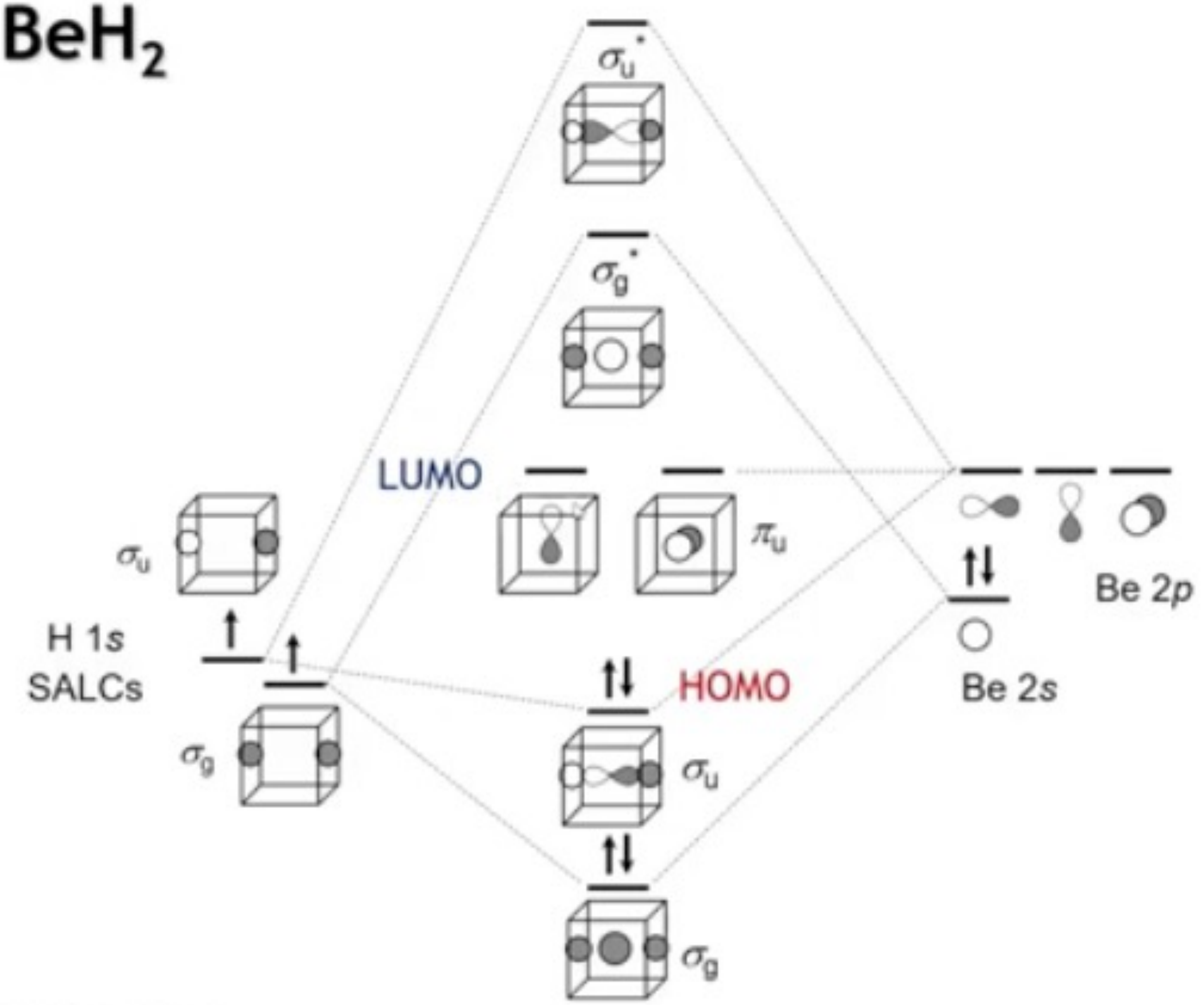


Treat the ligand orbitals as symmetry adapted linear combinations (SALCs)

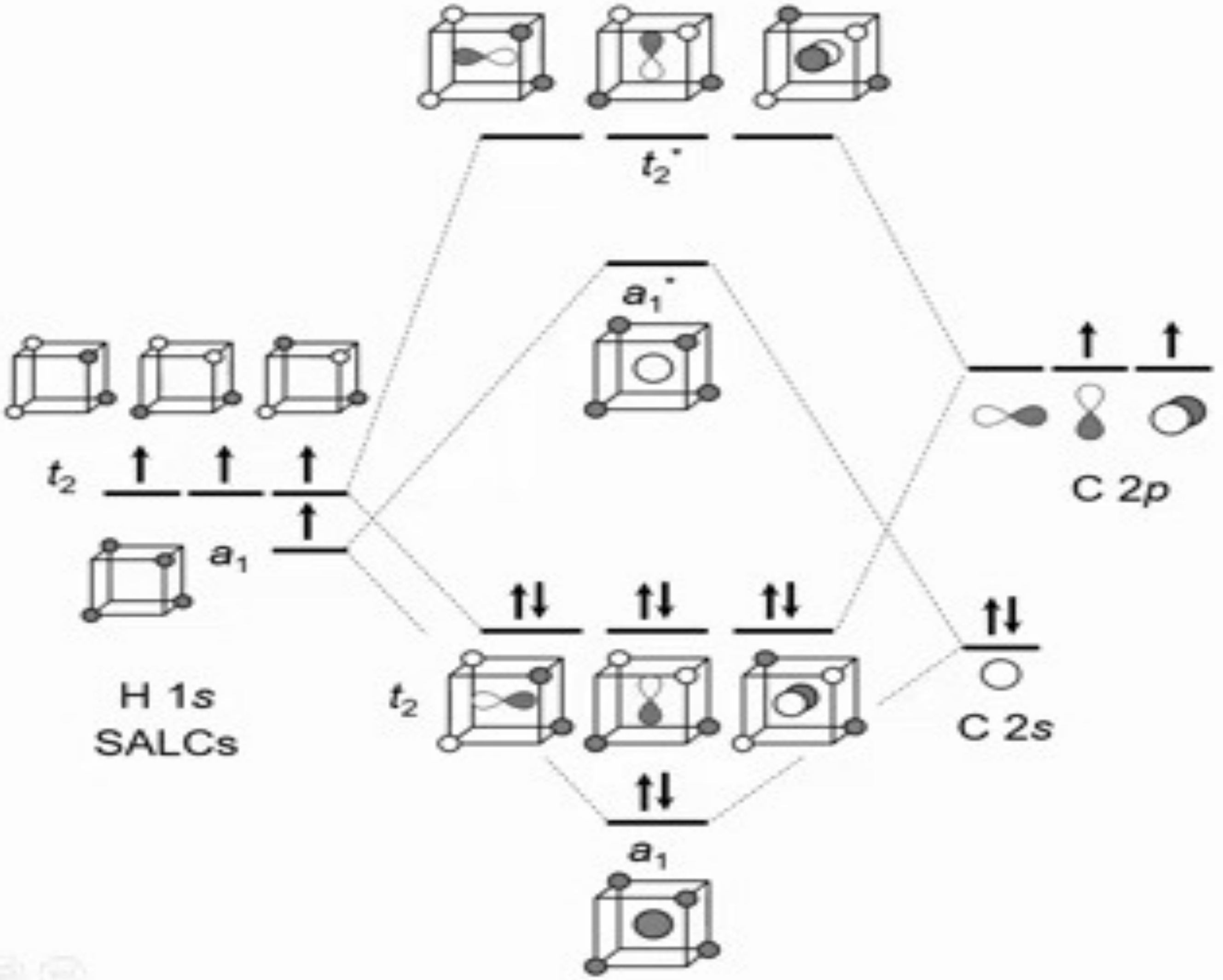
BeH$_2$



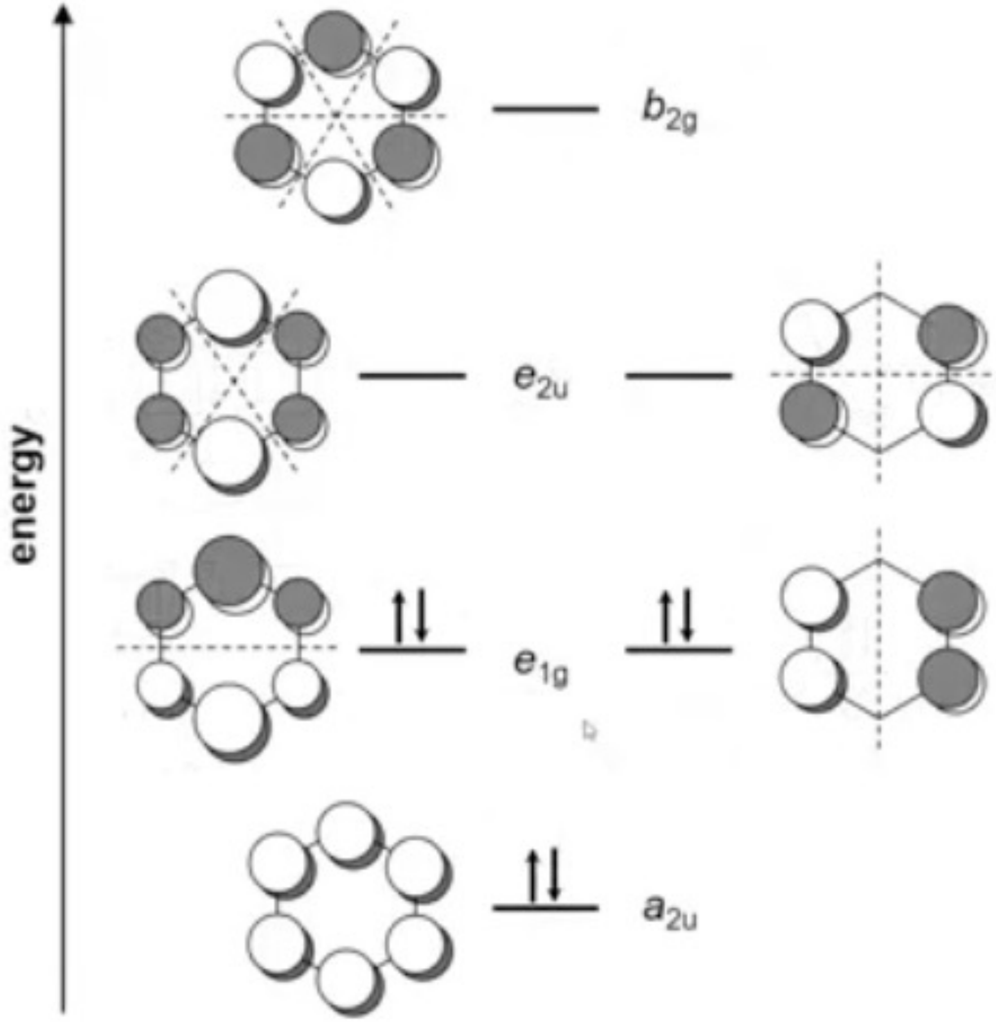
BeH$_2$


σ_u^*
σ_g^*
LUMO
π_u
σ_u
H 1*s*
SALCs
σ_g
Be 2*p*
Be 2*s*
HOMO
σ_u
σ_g

CH$_4$



Delocalized pi-bonding in benzene



Summary — Molecular Orbital Theory

- Molecular orbitals (MOs) form from **linear combinations of atomic orbitals (LCAO)**; electrons are described by delocalized wave functions over the entire molecule.
- **Bonding MOs** arise from constructive interference (increased electron density between nuclei → stabilization).
- **Antibonding MOs** arise from destructive interference (nodal plane between nuclei → destabilization).
- Energy splitting between bonding and antibonding orbitals increases with **orbital overlap** and decreases with **energy mismatch**.
- **Polarity** arises when orbitals of unequal energy mix, giving partial ionic character.
- **σ and π bonds** differ by overlap geometry: σ bonds form along the internuclear axis, π bonds form side-on.
- **s–p mixing** alters MO energy ordering, notably in lighter diatomics (C_2, N_2).
- For polyatomic molecules, **ligand orbitals combine into SALCs** that mix with central-atom orbitals of matching symmetry.
- **HOMO and LUMO** define the frontier orbitals controlling reactivity and optical transitions.
- In **conjugated π systems**, delocalization spreads bonding over many atoms, producing evenly spaced energy levels (e.g., benzene).

Homework: 5.7 – 5.13, 5.15