

43384 – Digital Alchemy

Unit 01 – General Chemistry

Prof. Dr. Carolin Müller

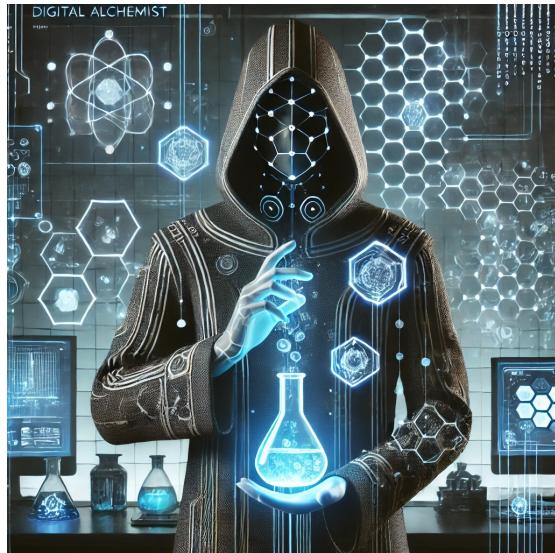
October 13, 2025

Alchemy

- An ancient philosophical and proto-scientific tradition (blend of chemistry, metaphysics, and spirituality), laying the groundwork for modern chemistry.
- Its goals included the transmutation of base metals into gold, the discovery of the philosopher's stone, and the pursuit of immortality.
- **Alchemists sought to transform matter.**

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(generated with DALL·E)

Digital Alchemy

- Digital Alchemy utilizes cheminformatics, machine learning, and in silico simulations to:
 - **Predict chemical properties** and reactions.
 - Design new molecules and materials.
 - Explore vast chemical spaces that are otherwise inaccessible experimentally.
- Digital alchemists seek to **transform data into valuable insights and discoveries in chemistry**.

Overview Digital Chemistry

Topics, Flipped Classroom, Project & Exam

Lecture + Hands-On:

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1. General Chemistry (13.10.)

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bold dates: Tuesday

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3. Searching Chemical Structures (**04.11.**)

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Individual projects:

- self-study (paper-presentation, project pitch):
 - 24.11. & 01.12.2025

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 - 22.12.2025 – 06.02.2026
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 - 22.12.2025 – 06.02.2026
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 - final report ('examination' object) to be submitted by **09.02.2026**

Getting to Know Each Other

Introduce yourself:

1. Your **name**

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2. Your **scientific background**
(e.g. Data Science, Engineering, etc.)

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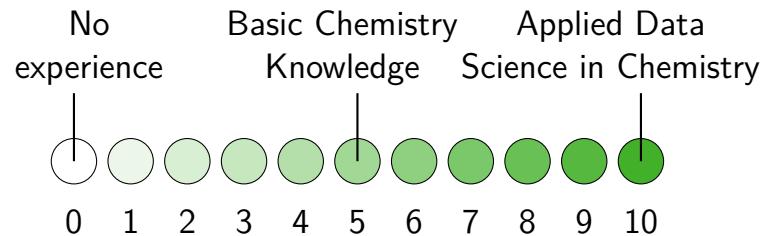
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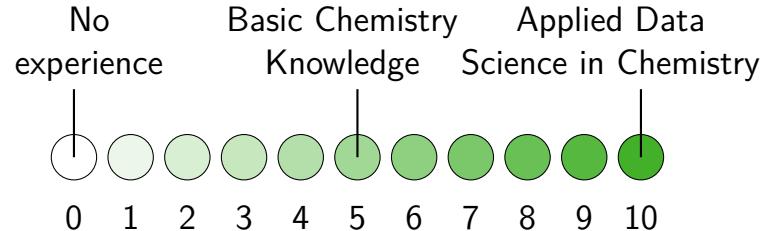


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- Pick a familiar library from the grid

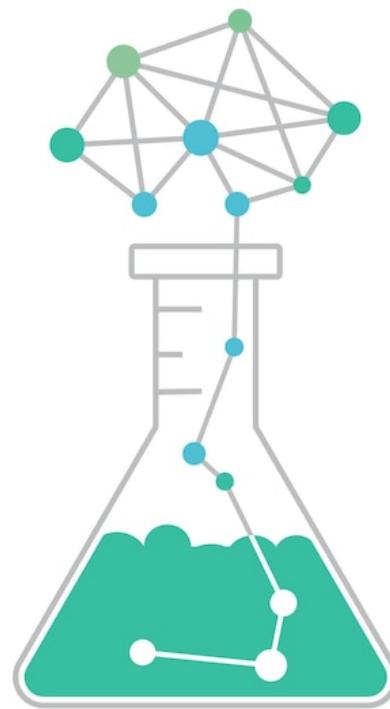


numpy	seaborn	scipy	pandas	rdkit
sklearn	numpy	networkx	pybel	<i>matplotlib</i>
<i>seaborn</i>	scipy	ase	numpy	networkx
<i>matplotlib</i>	veloxchem	pandas	<i>seaborn</i>	numpy
openbabel	pandas	sklearn	<i>matplotlib</i>	<i>seaborn</i>

Data Science & Chemistry

Data scientists model entities, relationships, and constraints.

Chemists do the same — just with molecules (atoms and bonds) and their properties.

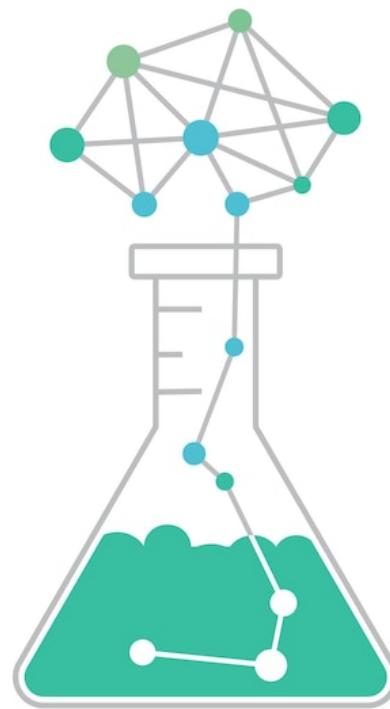


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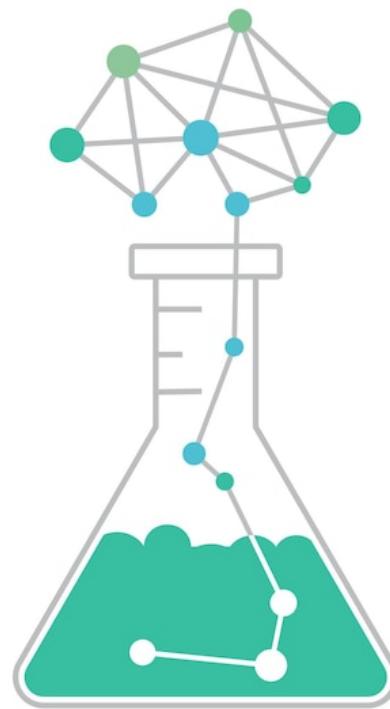


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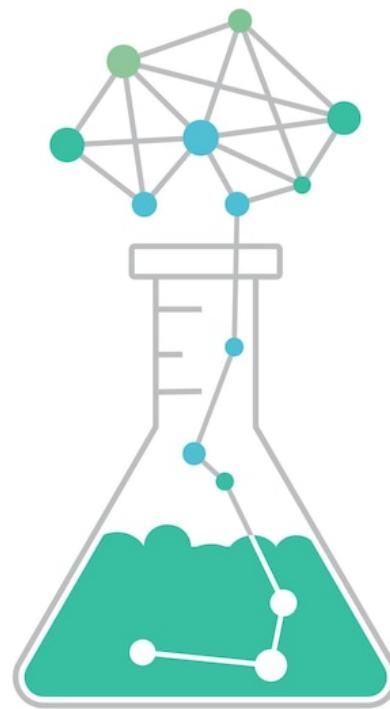


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 - Rules and constraints (valence of atoms = invariants)
 - Patterns and generalizations (Functional groups, substructures = templates)



1. Basic Terms

2. Atoms

2.1 Bohr's Atom Model

2.2 Schrödinger Wave Equation

2.3 Atomic Orbitals

3. Molecules

3.1 Types of Bonding

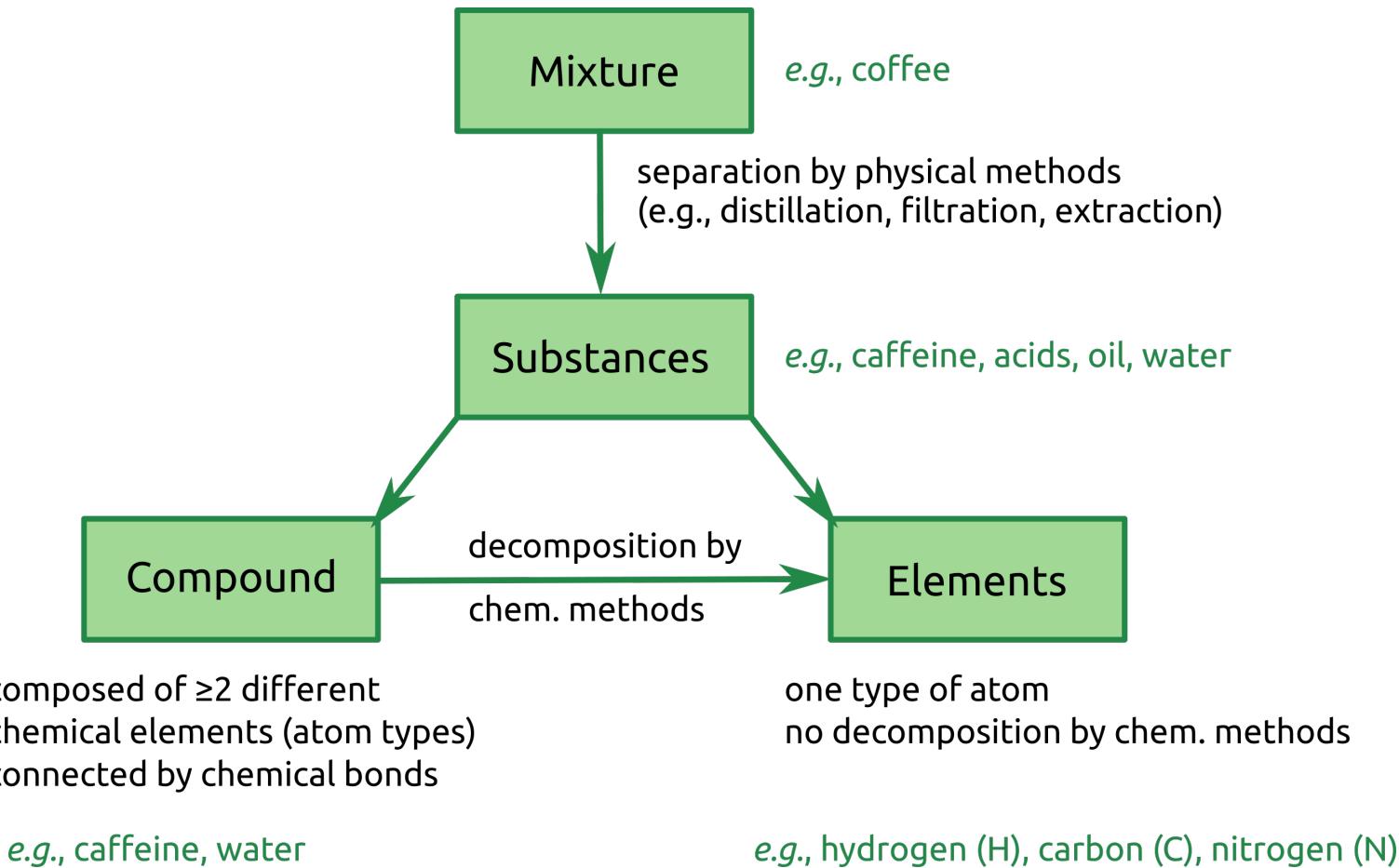
3.2 Valence Bond Theory

3.3 Hybridization

3.4 Molecular Orbital Theory

Hierarchy of Matter

Mixtures, Substances, Compounds, Elements



Symbols of Chemical Elements

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Symbols used for abbreviation of chemical elements by elements by Berzelius; today by IUPAC: One- or two-letters long, only first capitalized. Mostly derived from Greek or Latin words.

1	H	Hydrogen
2	He	Helium
3	Li	Lithium
4	Be	Beryllium
5	B	Boron
6	C	Carbon
7	N	Nitrogen
8	O	Oxygen
9	F	Fluorine
10	Ne	Neon

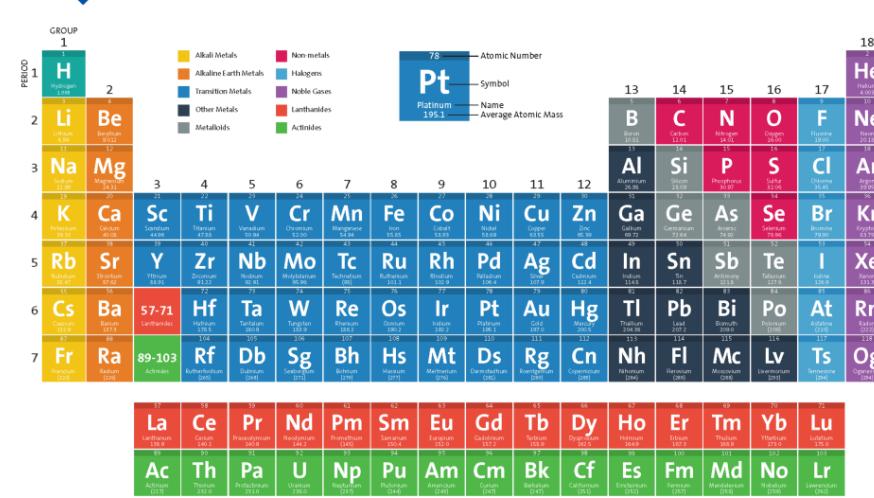


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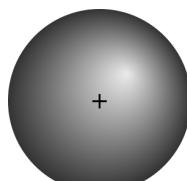
American Chemical Society

[www.acs.org/outreach](http://acs.org/outreach)

Elementary particle

Atoms are composed of three fundamental particles:

Particle	Electric Charge	Mass (relative)	Location
proton	+1	1	nucleus
neutron	0	1	nucleus
electron	-1	$\frac{1}{1800}$	in orbit around nucleus



proton



neutron

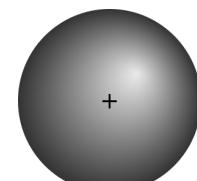


electron

Elementary particle

Atoms are composed of three fundamental particles:

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proton	+1	1	nucleus
neutron	0	1	nucleus
electron	-1	$\frac{1}{1800}$	in orbit around nucleus



proton



neutron



electron

Atomic Notation



where:

- A = mass number = protons + neutrons
- Z = atomic number = protons
- X = element symbol

Example:



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2.2 Schrödinger Wave Equation

2.3 Atomic Orbitals

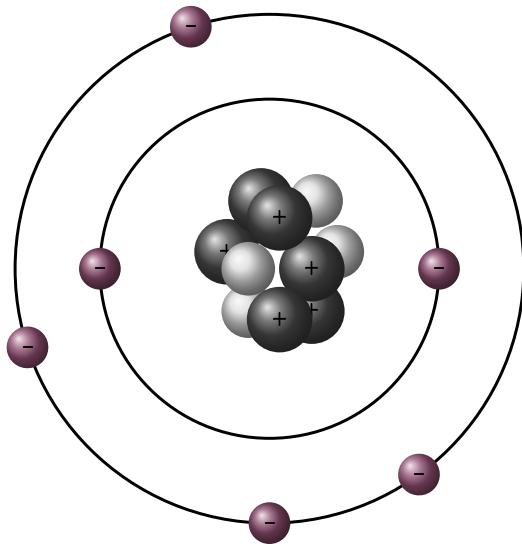
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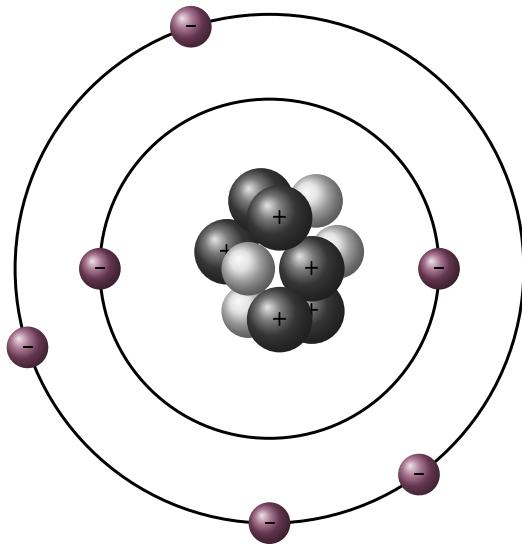
3.4 Molecular Orbital Theory



Bohr's Postulates

- 1) The **energy** of an electron in an atom can only have discrete values.

$$E_n \ (n = 1, 2, 3, \dots)$$



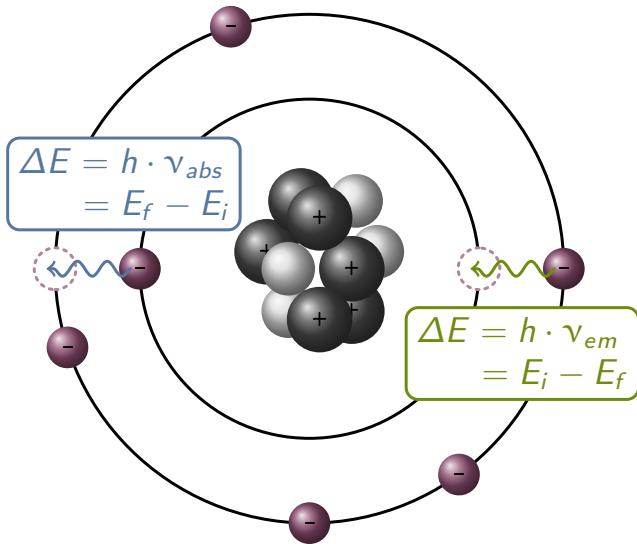
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$$E_n \quad (n = 1, 2, 3, \dots)$$

2) Electrons move radiation-free (without energy loss) and with a **constant speed** \vec{v}_n at a **fixed distance** \vec{r}_n around the atomic nucleus. The angular momentum of the revolving electron is an integer multiple of the reduced Planck constant:

$$m_e \cdot \vec{v}_n \cdot 2\pi \vec{r}_n = n \cdot \hbar$$



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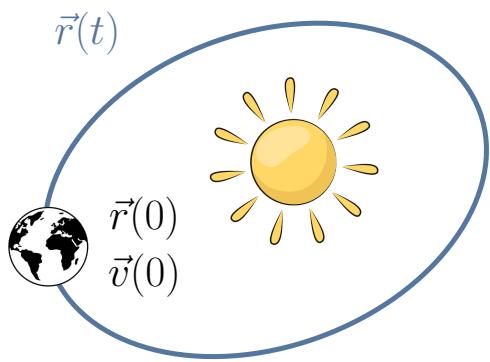
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3) Electrons can only absorb or emit energy by **jumping** from one allowed orbit to another. Absorbing or emitting electromagnetic radiation with a frequency ν is determined by the energy difference of the respective two energy levels:

$$\Delta E = |E_f - E_i| = h \cdot \nu$$



$$\vec{F} = m \cdot \vec{a}$$
$$-\nabla E_{\text{pot}} = m \frac{d^2 \vec{r}(t)}{dt^2}$$

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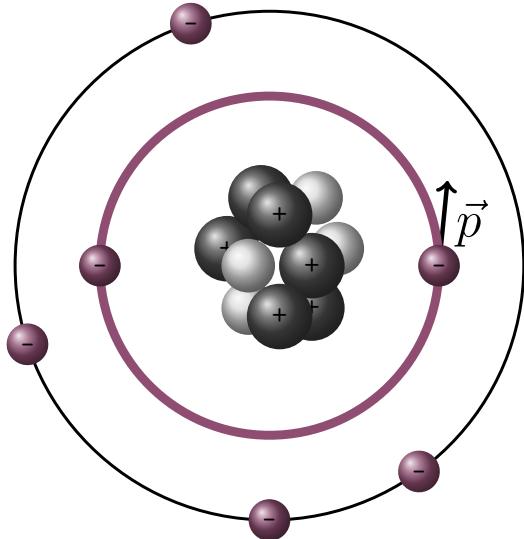
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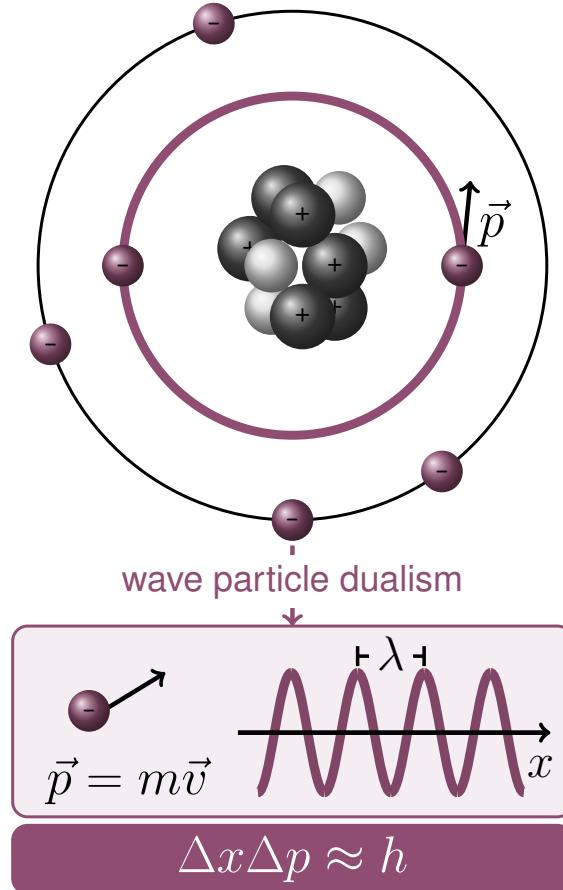
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Limits of Bohr's Model



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1D-Schrödinger wave equation (SE)

Time-dependent and stationary SE

- time-dependent SE:

$$i\hbar \frac{\partial}{\partial t} \Psi(x, t) = \hat{H}\Psi(x, t) = \hat{T}\Psi(x, t) + \hat{V}\Psi(x, t)$$

$$i\hbar \frac{\partial}{\partial t} \Psi(x, t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Psi(x, t) + V(x)\Psi(x, t)$$

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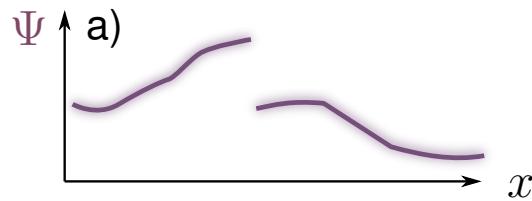
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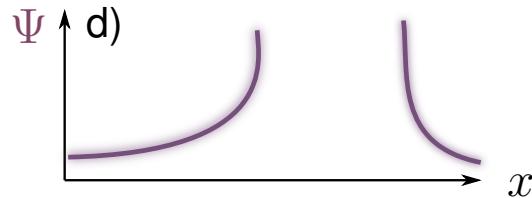
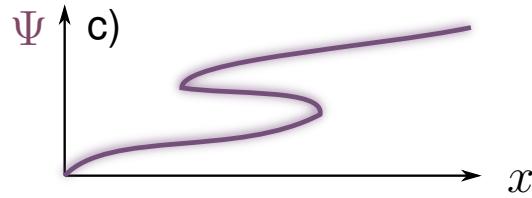
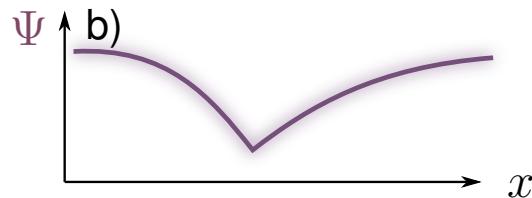
$$0 = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Psi(x) + V(x)\Psi(x) = E\Psi(x)$$

Solution of SE: Wave functions

Properties of the wave function

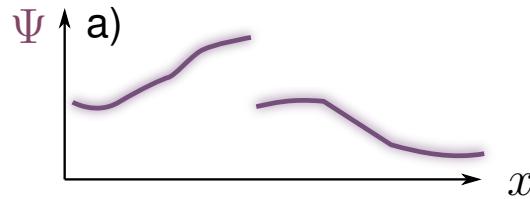


→ **discontinuous** function

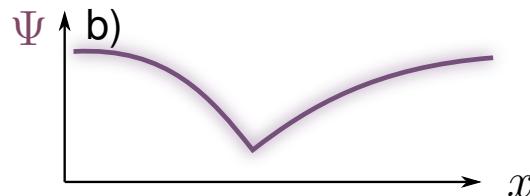


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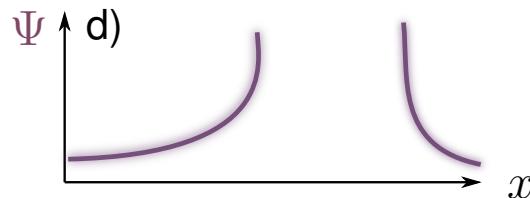
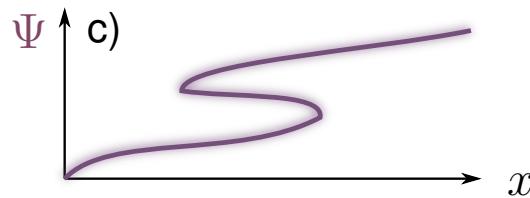
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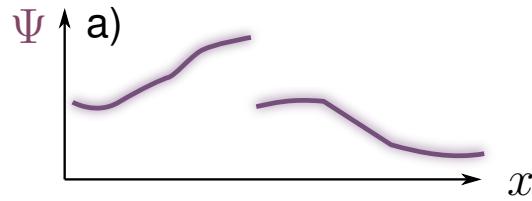


→ function with **discontinuous 1st derivative**

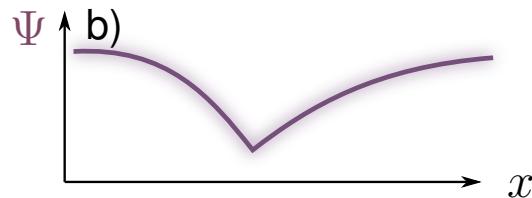


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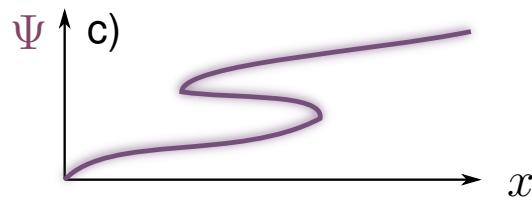
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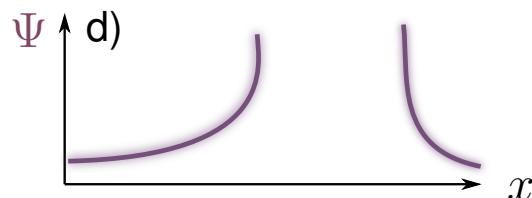
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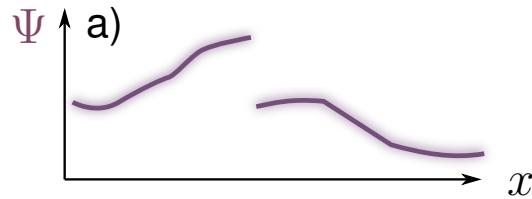


→ function is **not unique** with regard to x

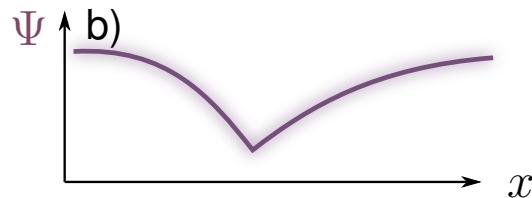


Solution of SE: Wave functions

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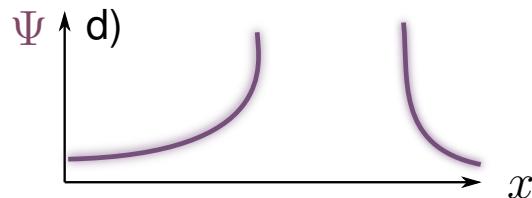
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→ function with **discon-**
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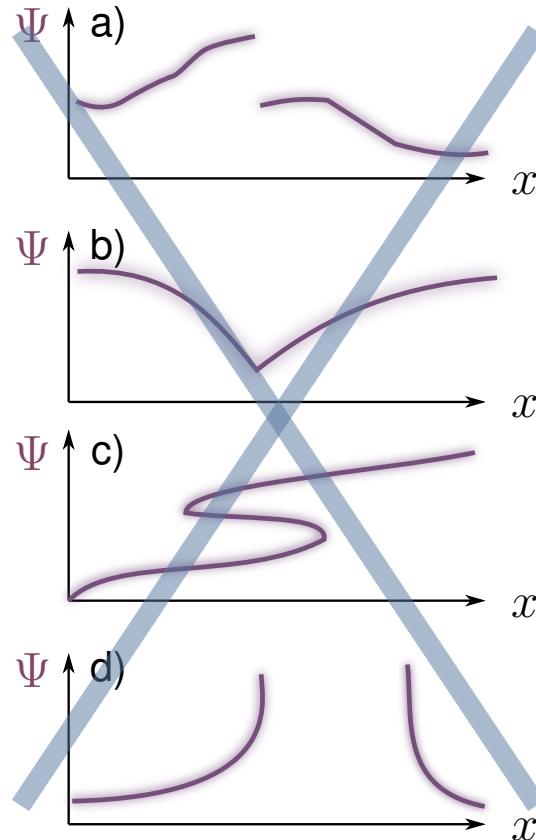
→ function is **not unique**
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→ function is **infinite** in
the finite domain

Solution of SE: Wave functions

Properties of the wave function



→ **discontinuous** function
not allowed!

→ function with **discon-**
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not allowed!

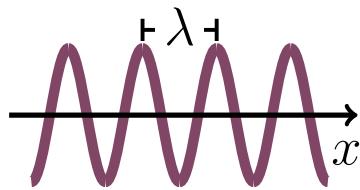
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→ function is **infinite** in
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The wave function Ψ needs to be **continuous**, have a **continuous 1st derivative**,
be **unique** with respect to x , and be **finite**.

Solution of SE: Wave functions

Classical wave theory and wave functions



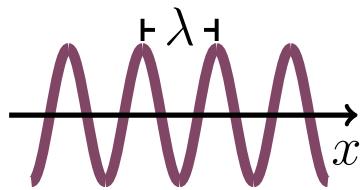
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↑ amplitude ↑ wave vector

The wave function $\Psi(x)$ needs to be **continuous**, have a **continuous 1st derivative**, be **unique** with respect to x , and be **finite**.

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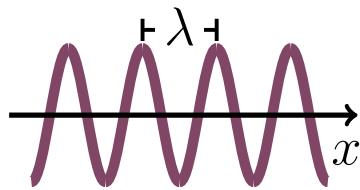
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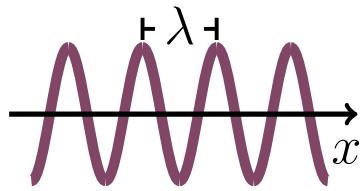
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Solution of SE: Wave functions

Classical wave theory and wave functions



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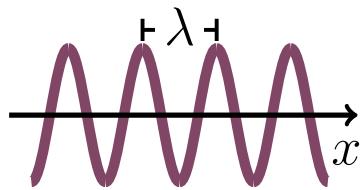
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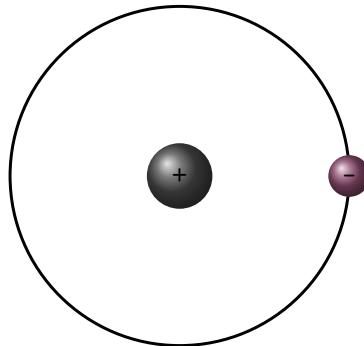
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Hamiltonian \hat{H} contains two main contributions:

- **Electron kinetic energy (\hat{T})**: Represents the motion of the electron in space.
- **Coulomb potential (\hat{V})**: Attractive force between negatively charged electron and positively charged nucleus.

$$\begin{aligned}\hat{H} &= \hat{T} + \hat{V} \\ &= -\frac{\hbar^2}{2m_e} \nabla^2 - \frac{k_e e^2}{r}\end{aligned}$$

Solution procedure in a nutshell:

- Use *spherical coordinates* (r, θ, ϕ) .
- Separate into radial part and angular part $\rightarrow \psi(r, \theta, \phi) = R(r) Y(\theta, \phi)$.
- Apply boundary conditions (wavefunction finite at $r = 0$ and vanishing at $r \rightarrow \infty$).

Atomic Orbitals

Solution of SE for Hydrogen-like Atoms

Atomic Orbitals

Atomic orbitals (AOs) are solutions of the Schrödinger equation for the hydrogen-like atom. Each atomic orbital is a product of a radial ($R_{n,l}(r)$) and angular function ($Y_{l,m}(\theta, \phi)$):

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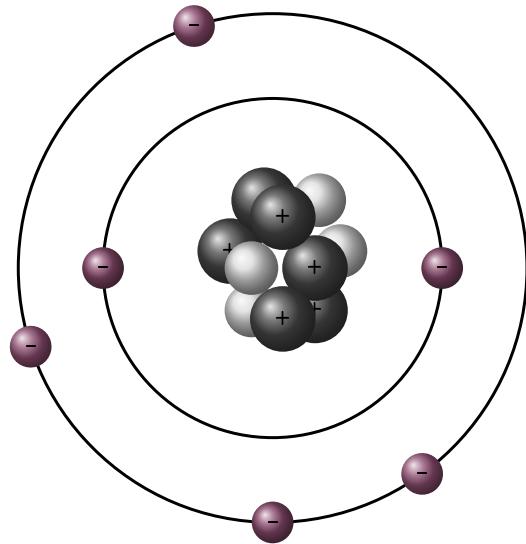
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- **magnetic quantum number (m_l)**: describes the orientation of the orbital in space ($m_l \in -l, -l + 1, \dots, l - 1, l$), e.g. $l = 1$ gives $m_l = -1, 0, 1 \rightarrow$ 3 different oriented p-orbitals

Atomic Orbitals

Shells, Subshells, and Orbitals

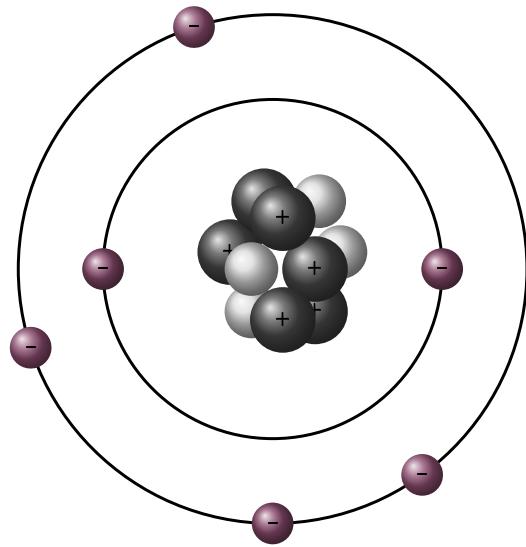


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Atomic Orbitals

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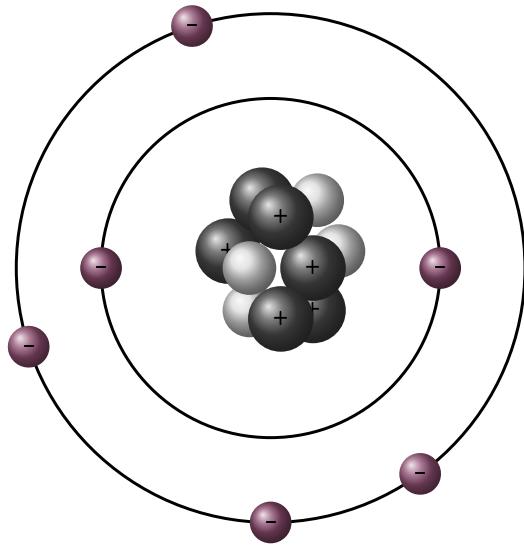
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- a set of orbitals with the same n and l values, e.g. second shell: $n = 2, l = 0, 1 \rightarrow 2$ subshells (2s and 2p)
- # of subshells within a shell is equal to n
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- **Orbitals:**

- regions within a subshell where electrons are likely to be found
- each orbital can hold a maximum of 2 electrons (with opposite spins)
- number of orbitals in a subshell is $2l + 1$

Atomic Orbitals

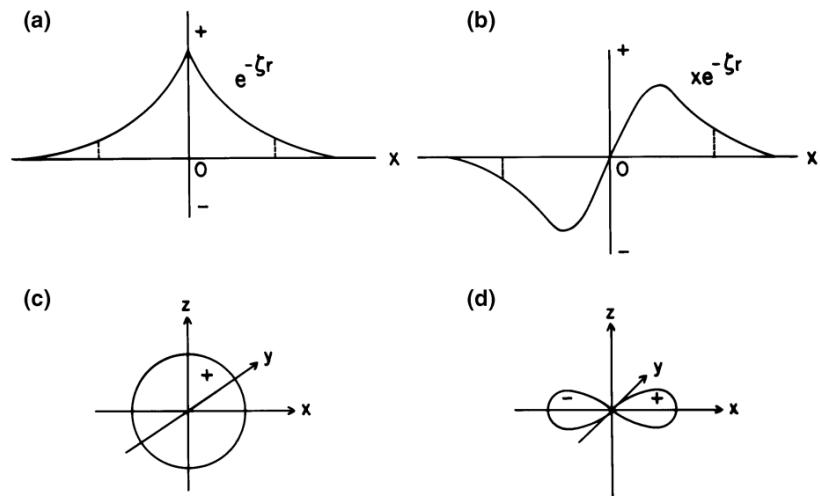
Types of atomic orbitals

General Form:

$$\psi_{n,l,m}(r, \theta, \phi) = R_{n,l}(r) Y_{l,m}(\theta, \phi)$$

Examples for common orbitals:

Orbital	Radial Part $R_{n,l}(r)$	Angular Part $Y_{l,m}(\theta, \phi)$
1s	$2e^{-r/a_0}$	$\frac{1}{\sqrt{4\pi}}$
2p _x	$\frac{1}{2\sqrt{6}a_0^{3/2}} \left(\frac{r}{a_0}\right) e^{-r/2a_0}$	$\sqrt{\frac{3}{4\pi}} \sin \theta \cos \phi$
2p _y	same radial as 2p _x	$\sqrt{\frac{3}{4\pi}} \sin \theta \sin \phi$
2p _z	same radial as 2p _x	$\sqrt{\frac{3}{4\pi}} \cos \theta$
3d _{xz}	$\frac{4}{81\sqrt{30}a_0^{3/2}} \left(\frac{r^2}{a_0^2}\right) e^{-r/3a_0}$	$\sqrt{\frac{15}{4\pi}} \sin \theta \cos \theta \cos \phi$

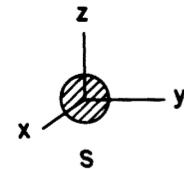


Atomic Orbitals

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- **s-orbitals:**

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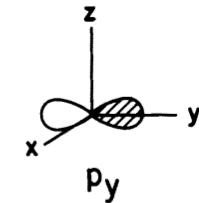
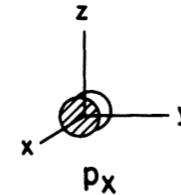
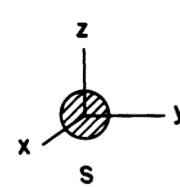


Atomic Orbitals

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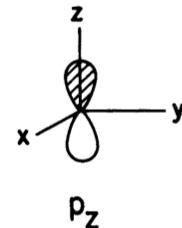
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- there are 3 iso-energetic p-orbitals per energy level oriented along x, y and z-axis (same size and shape)

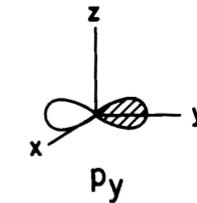
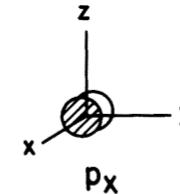
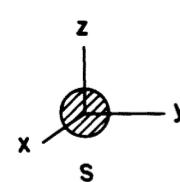


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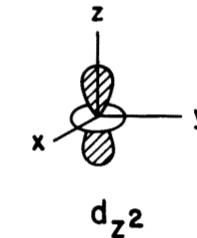
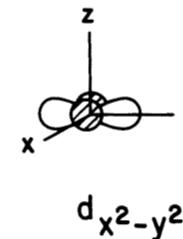
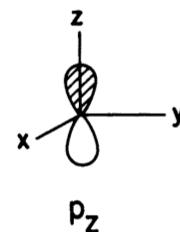
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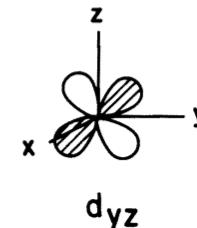
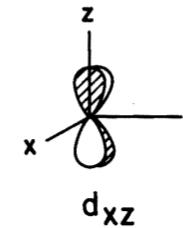
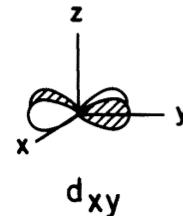
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- there are 5 iso-energetic d-orbitals per energy level



Electronic Structure Principles

Pauli, Aufbau and Hund principle

- **Pauli exclusion principle:**

- 2 electrons in an atom cannot have the same set of 4 quantum numbers (n , l , m_l , m_s), e.g., maximum of 2 electrons in the 1s orbital

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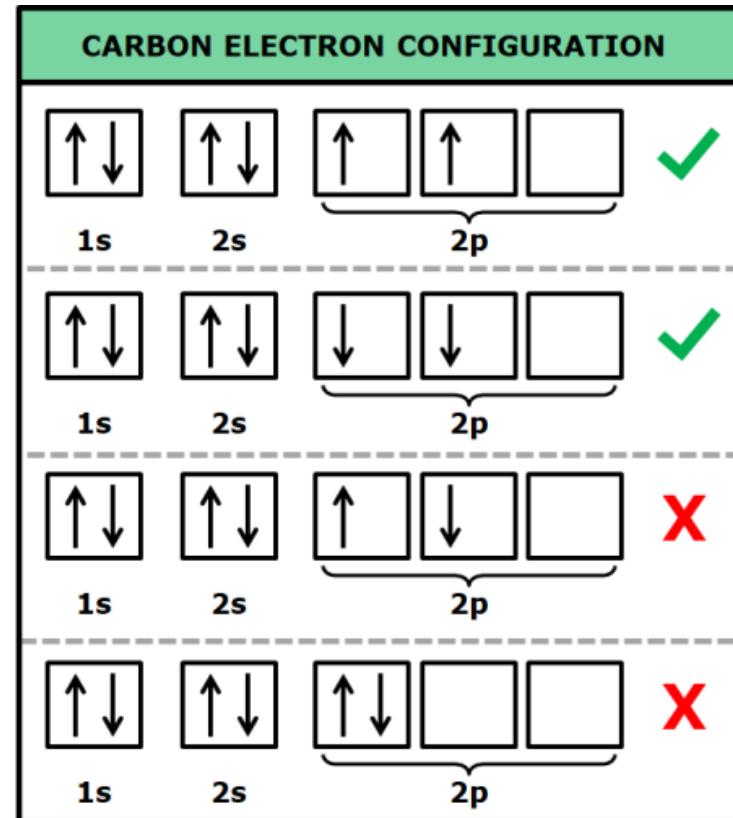
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- **Core electrons:** Inner-shell electrons corresponding to the configuration of the previous noble gas. ⇒ Chemically inert, shield the nucleus.
- **Valence electrons:** Outermost electrons (highest n) involved in chemical bonding and reactivity.

1. Basic Terms

2. Atoms

2.1 Bohr's Atom Model

2.2 Schrödinger Wave Equation

2.3 Atomic Orbitals

3. Molecules

3.1 Types of Bonding

3.2 Valence Bond Theory

3.3 Hybridization

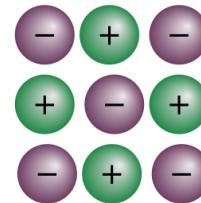
3.4 Molecular Orbital Theory

Types of Bonding

The properties of substances are determined by the type of bonding within the substance. There are 3 main types of bonding:

- **Ionic bonds:**

- Ionic bonds are formed between a metal cation and a non-metal anion due to the electrostatic force that binds ions of opposite charge. This type of bond results from the complete transfer of one or more electrons from one atom to another, leading to the formation of 2 charged particles, called ions.

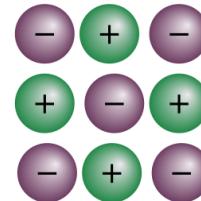


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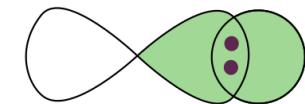
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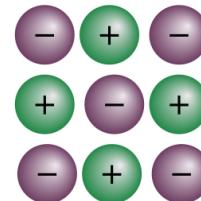


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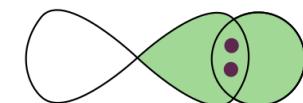
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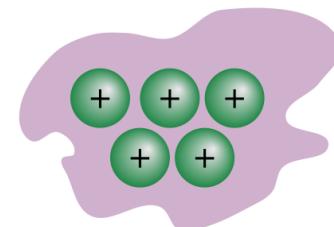
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Covalent Bonding

Covalent Compounds

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each chlorine atom has 7 electrons in its outer shell

each chlorine atom has 8 electrons in its outer shell

The Octet Rule

Covalent Compounds

Octet Rule

Main-group elements tend to form molecules by **gaining, losing, or sharing electrons** to achieve a stable configuration with **eight electrons in their valence shell**, resembling the noble gases.

- Explains bonding patterns of second-period elements (C, N, O, F).
- Foundational for understanding molecular structure and organic reactivity.

The Octet Rule

Covalent Compounds

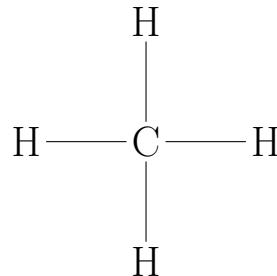
Octet Rule

Main-group elements tend to form molecules by **gaining, losing, or sharing electrons** to achieve a stable configuration with **eight electrons in their valence shell**, resembling the noble gases.

- Explains bonding patterns of second-period elements (C, N, O, F).
- Foundational for understanding molecular structure and organic reactivity.

Carbon (C)

- $Z = 6 \Rightarrow 1s^2 2s^2 2p^2 \Rightarrow 4$ valence electrons.
- Needs 4 more electrons \rightarrow forms **4 covalent bonds** (tetra-valent).
- Example: Methane, CH_4



The Octet Rule

Covalent Compounds

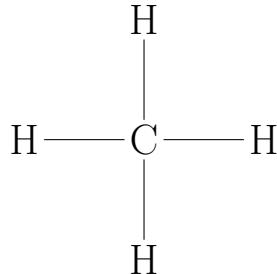
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- Example: Methane, CH_4



Oxygen (O)

- $Z = 8 \Rightarrow 1s^2 2s^2 2p^4 \Rightarrow 6$ valence electrons.
- Needs 2 more electrons \rightarrow forms **2 covalent bonds**.
- Example: Water, H_2O



Definition

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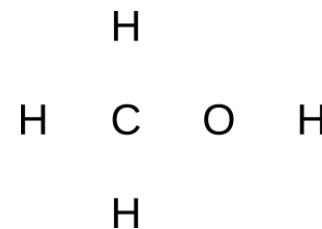
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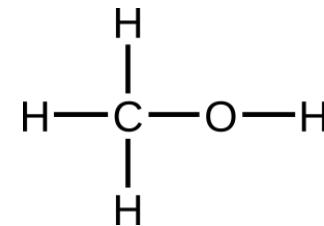
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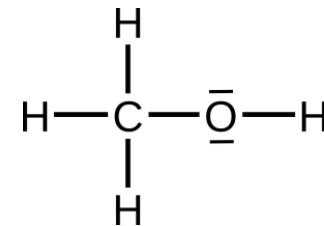
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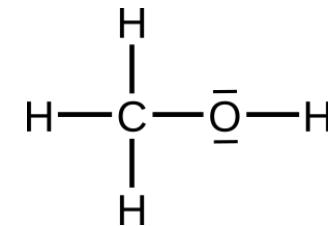
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5. Use double or triple bonds if needed to satisfy octet.
6. Verify total electron count and assign formal charges:

$$\text{Formal charge} = (\text{valence } e^-) - (\text{nonbonding } e^-) - \frac{1}{2}(\text{bonding } e^-)$$

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- Carbon: 4 valence electrons
- Hydrogen: 1 valence electron ($\times 4$)
- Oxygen: 6 valence electrons
- Total valence electrons: $14 \rightarrow 7$ bonds



Molecular Shape

Lewis Structures and VSEPR

Molecular shape determines key properties such as **reactivity, polarity, color, and biological activity**.

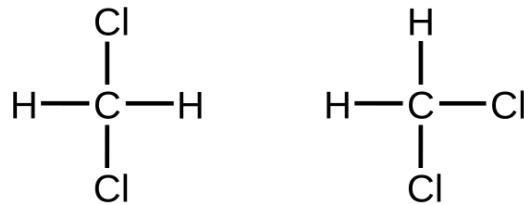
From Lewis structures to geometry:

Lewis structures show how atoms connect and share electrons, but they do **not** indicate the 3D orientation of bonds. To predict shape, we use **VSEPR theory**, which considers electron-pair repulsion around the central atom.

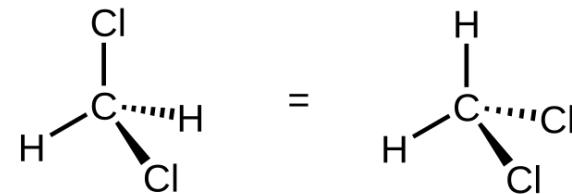
Steps to determine shape:

1. Draw the Lewis structure.
2. Count electron domains (bonding + lone pairs).
3. Apply **VSEPR** to predict 3D geometry.

2 Lewis structures



1 molecule



Molecular Shape

Lewis Structures and VSEPR

VSEPR Theory (Valence-Shell Electron-Pair Repulsion):

- Predicts molecular shape from **repulsion between electron pairs** (bonding and lone pairs) around the central atom.
- Electron pairs arrange to **minimize repulsion** → maximize distance.

Molecular Shape

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VSEPR notation: AX_nE_m

- A : central atom
- X : surrounding atoms (n)
- E : lone pairs on central atom (m)

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Domains	Geometry	Example	Angle
2	Linear (AX_2)	CO_2	180°

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Molecular Shape

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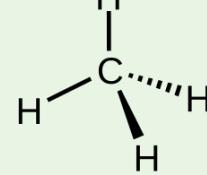
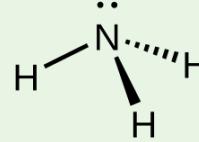
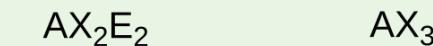
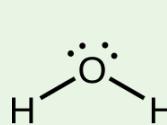
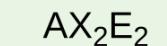
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Domains	Geometry	Example	Angle
2	Linear (AX_2)	CO_2	180°
3	Trigonal planar (AX_3)	BF_3	120°
	Bent (AX_2E)	SO_2	$\sim 118^\circ$
4	Tetrahedral (AX_4)	CH_4	109.5°
	Trigonal pyramidal (AX_3E)	NH_3	$\sim 107^\circ$
	Bent (AX_2E_2)	H_2O	$\sim 104.5^\circ$

VSEPR notation: AX_nE_m

- A : central atom
- X : surrounding atoms (n)
- E : lone pairs on central atom (m)

Examples



bent

trigonal pyramidal

tetrahedral

Bonding theories

Valence Bond Theory

Bonding theories:

- Lewis structures and **VSEPR theory** predict molecular geometry but not *how* bonds form.
- Two main bonding theories explain bond formation:
 - **Valence Bond Theory (VBT)**: Bonds form when atomic orbitals overlap.
 - **Molecular Orbital Theory (MOT)**: Treats bonding with delocalized molecular orbitals derived from atomic orbitals.

Core idea of Valence Bond Theory:

- Atoms share electrons via overlap of partially filled **atomic orbitals (AOs)**.
- A bond forms if the resulting molecule has **lower energy** than the separated atoms.
- **Bond strength** \propto extent of orbital overlap.
- bond types:
 - **s-orbital bonds**: non-directional.
 - **p, d, f-orbital bonds**: directional \Rightarrow determine molecular geometry.
- Lower energy state:
 - The formation of a covalent bond via orbital overlap results in a molecule with a lower potential energy compared to the separate atoms, making the bonded state more stable.

Single and Multiple Bonds

σ and π -Bonds

Bond Types

- **σ -bond:**
 - Formed by **head-on overlap** of orbitals along the internuclear axis.
 - Overlap can occur between two s orbitals, an s- and a p-orbital, or two p-orbitals.
 - Allows **free rotation** around the bond axis.



s-s overlap
e.g. H₂



s-p overlap
e.g. HCl



p-p overlap
e.g. Cl₂

Single and Multiple Bonds

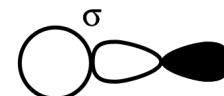
σ and π -Bonds

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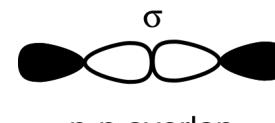
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 - Formed by **side-by-side overlap** of two parallel p orbitals.
 - Electron density lies **above and below** the internuclear axis.
 - **Restricts rotation** due to the nature of the overlap.



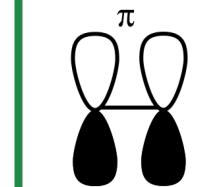
s-s overlap
e.g. H₂



s-p overlap
e.g. HCl



p-p overlap
e.g. Cl₂



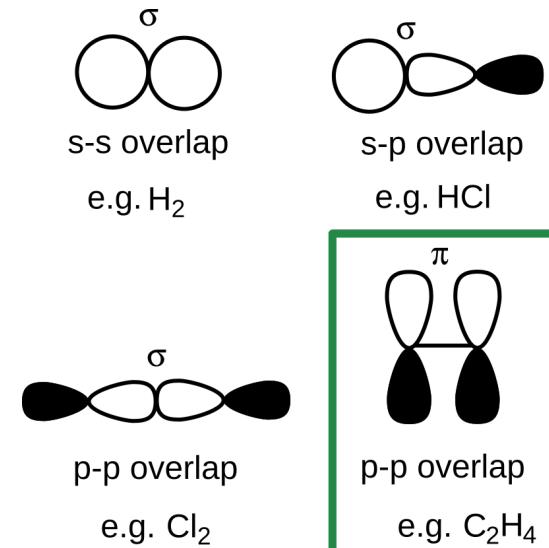
π
p-p overlap
e.g. C₂H₄

Single and Multiple Bonds

σ and π -Bonds

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Types of covalent bonds:

- **Single bond:** 1 σ bond (2 e^- shared)
- **Double bond:** 1 σ + 1 π bond (4 e^-); planar; restricted rotation
- **Triple bond:** 1 σ + 2 π bonds (6 e^-); linear; no rotation

Hybrid Orbitals

Hybridization

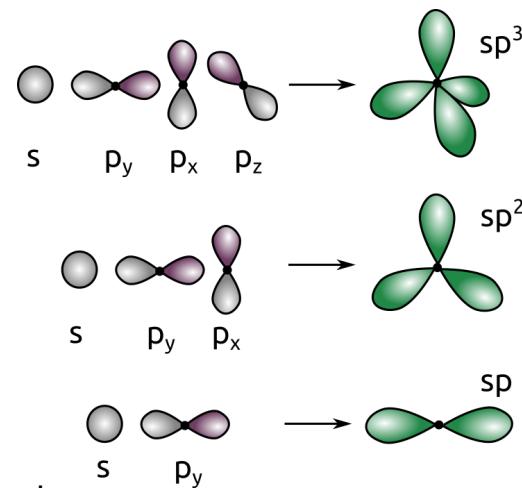
To explain bonding in some molecules, we must use the concept of hybridization, where two or more atomic orbitals combine to form the same number of hybrid orbitals with new energies and shapes. Hybridization helps in understanding the geometry and bonding properties of molecules.

Hybrid orbitals from s- and p-orbitals:

Type	Orbitals Used	Bonds Formed	Geometry	Example
sp^3	1s + 3p	4 σ	tetrahedral	CH_4
sp^2	1s + 2p	3 σ , 1 π	trigonal planar	C_2H_4
sp	1s + 1p	2 σ , 2 π	linear	C_2H_2

analogy to data science:

- hybridization = feature transformation
- raw orbitals (s, p) \rightarrow hybrid orbitals (sp^n) = new basis better suited for bonding = Like transforming a basis in linear algebra to align with system symmetry



Molecular Orbital Theory

The LCAO Approach

Concept

- In Molecular Orbital Theory, **atomic orbitals (AOs)** combine to form **molecular orbitals (MOs)** that extend over the entire molecule.
- This process is described by the **Linear Combination of Atomic Orbitals (LCAO)** approach:

$$\psi_{\text{MO}} = c_A \psi_A + c_B \psi_B$$

where c_A and c_B are coefficients describing the contribution of each AO.

- The number of MOs formed equals the number of AOs combined.
- Analogy to Data Science:
 - A molecular orbital = linear combination of basis functions.
 - Similar to constructing vectors from basis vectors in a vector space.

Molecular Orbital Theory

Bonding and Antibonding Molecular Orbitals

Formation from LCAO

When two atomic orbitals ψ_A and ψ_B combine:

$$\psi_1 = \phi_1 + \phi_2 \quad (\text{bonding, constructive interference})$$

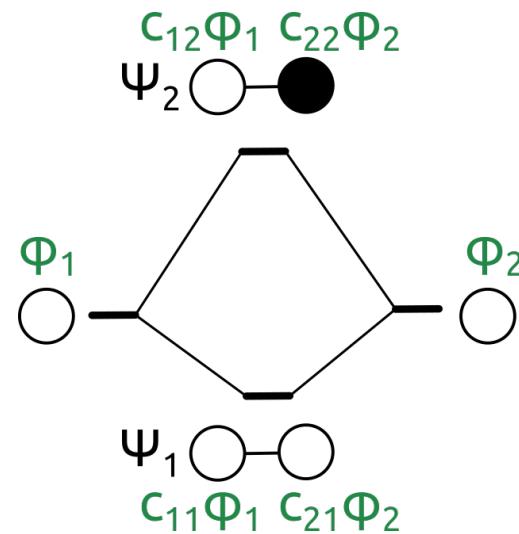
$$\psi_2 = \phi_1 - \phi_2 \quad (\text{anti-bonding, destructive interference})$$

Bonding Molecular Orbital:

- Electron density concentrated between nuclei.
- Constructive overlap \rightarrow lower energy than AOs.
- Stabilizes molecule.

Antibonding Molecular Orbital:

- Node between nuclei (no electron density).
- Destructive overlap \rightarrow higher energy than AOs.
- Destabilizes molecule.



Further Reading & Resources

- Textbooks (General Overviews):
 - Linus Pauling, *General Chemistry*
 - Peter Atkins, *Physical Chemistry*
- Online Resources and Practice:
 - **Introduction to Chemistry (Mark Bishop)** — free introductory material:
<http://preparatorychemistry.com/>
 - **Caltech Online Textbook (R. Dickerson)** — comprehensive general chemistry text:
<http://caltechbook.library.caltech.edu/178/>
 - **Chemistry Drills** – practice problems and quizzes: <http://www.chemistry-drills.com/>
 - **MIT OpenCourseWare – Chemistry** — lectures, notes, problem sets:
<https://ocw.mit.edu/courses/chemistry/>

Tip: For deeper dives into quantum chemistry, explore:

- *Quantum Chemistry* by Ira N. Levine
- *Orbital Interactions in Chemistry* by Thomas A. Albright, Jeremy K. Burdett & Myung-Hwan Whangbo

Next Steps: Learning Sequence on StudOn

- Open the course **learning sequence on StudOn**.
- First, you will see a page with the **lecture slides**.
- After reviewing the slides, you can attempt the **test**.

How to take the test:

- **On-site:** Complete the test in class. The lecturer is available to answer questions.
- **At home:** You can complete the test independently after further reading.

Tip: Review slides carefully, then attempt the questions actively – it will reinforce your understanding of molecular structure, bonding, and valence concepts.