Fundamentals of Solid State Physics

Preliminary Knowledge

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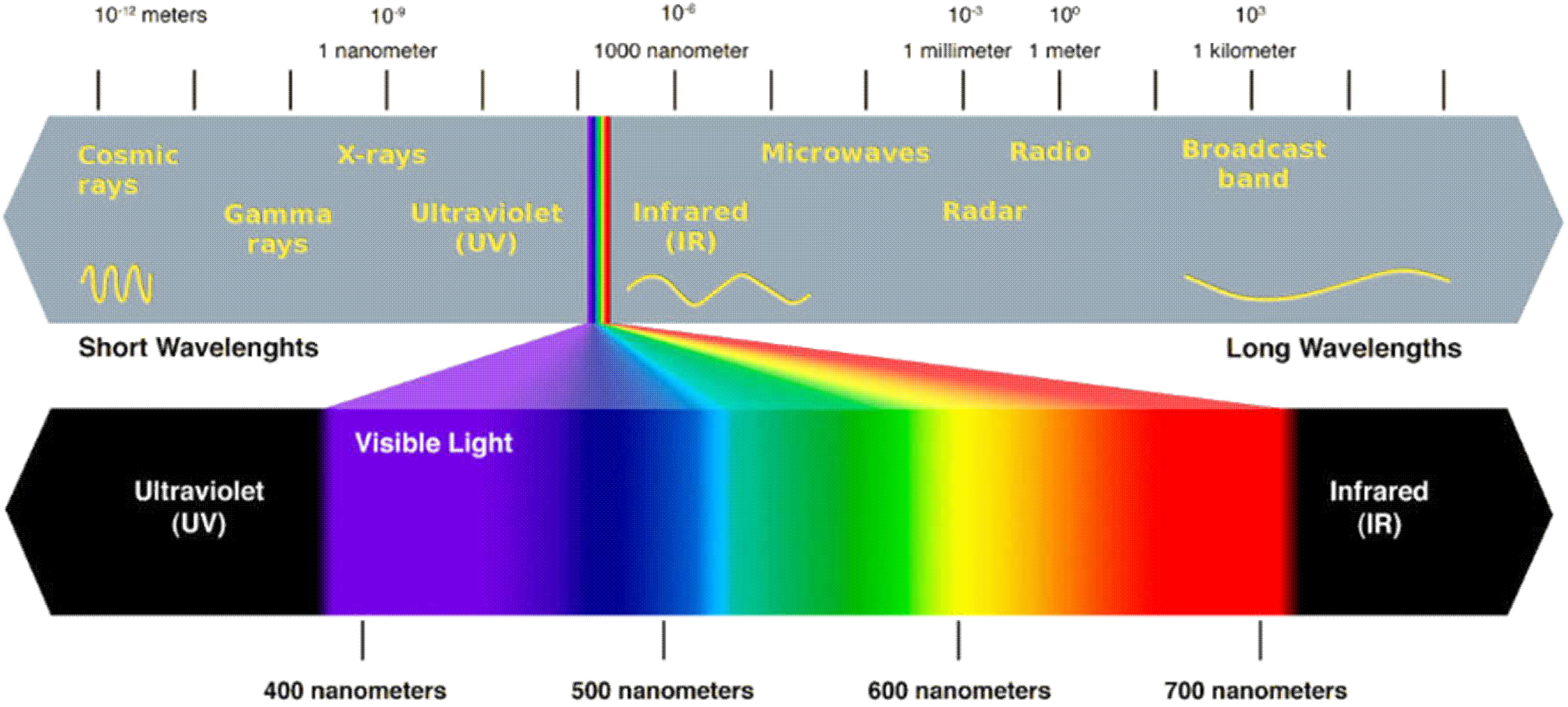
Preliminary Knowledge

- **Maths**
  - Calculus
  - Linear algebra
  - Probability and statistics
- **Physics**
  - Classical mechanics
  - Electrodynamics
  - Statistical mechanics
  - Quantum mechanics
- **Chemistry**
  - elements, atoms, molecules, bonding, ...

Table of Constants

Free electron mass	$m_e = 9.11*10^{-31}$ kg
Planck's constant	$h = 6.63*10^{-34}$ J s
Reduced Planck's constant	$\hbar = h/2\pi = 1.05*10^{-34}$ J s
Electron charge	$e = 1.6*10^{-19}$ C
Energy	1 eV = $1.6*10^{-19}$ J
Avogadro's number	$N_A = 6.02*10^{23}$ /mol
Boltzmann constant	$k_B = 1.38*10^{-23}$ J/K
Room temperature	$T = 300$ K
Speed of light in vacuum	$c = 3*10^{8}$ m/s
Permittivity of vacuum	$\varepsilon_0 = 8.85*10^{-12}$ F/m
Permeability of vacuum	$\mu_0 = 4\pi*10^{-7}$ H/m

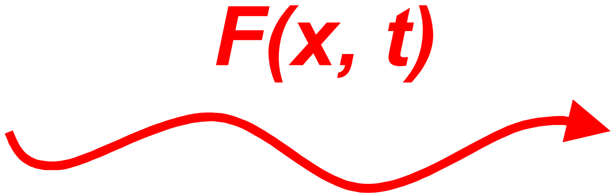
Optics



visible wavelength: 400–700 nm

Wave Functions

- Optical / Electromagnetic Wave
- Mechanical Wave
- Electron Wave
- ...



plane wave

$$\boxed{F(x,t) = Ae^{i(kx-\omega t+\varphi)}}$$

A - amplitude
k - wave vector (m^{-1})
ω - angular frequency (Hz)
φ - phase
ν - frequency (Hz)
T - period (s)
λ - wavelength (m)

$$\boxed{\omega = 2\pi\nu} \quad \boxed{T = \frac{1}{\nu}} \quad \boxed{k = \frac{2\pi}{\lambda}}$$

Photons

- **Photon Energy**

$$E = \hbar\omega = h\nu = h\frac{c}{\lambda}$$

- **Photon Momentum**

$$p = \frac{E}{c} = \frac{h}{\lambda}$$

- **Optical Wavelength**

$$\lambda = \frac{hc}{E} \rightarrow \lambda(\text{nm}) = \frac{1240}{E(\text{eV})}$$

E **(eV)**	λ **(nm)**
1	**1240**
2	**620**
3	**413**

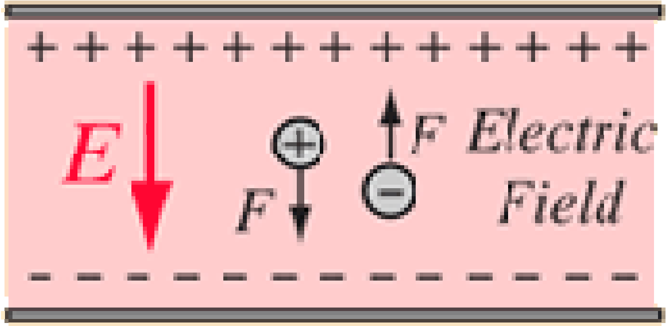
Electrons in Electromagnetic Fields

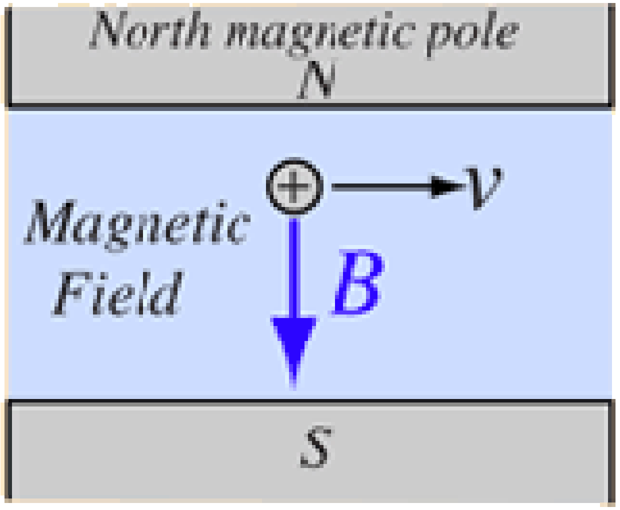
- **Lorentz force**

$$\boxed{\mathbf{F} = q\mathbf{E} + q\mathbf{v} \times \mathbf{B}}$$

electric force

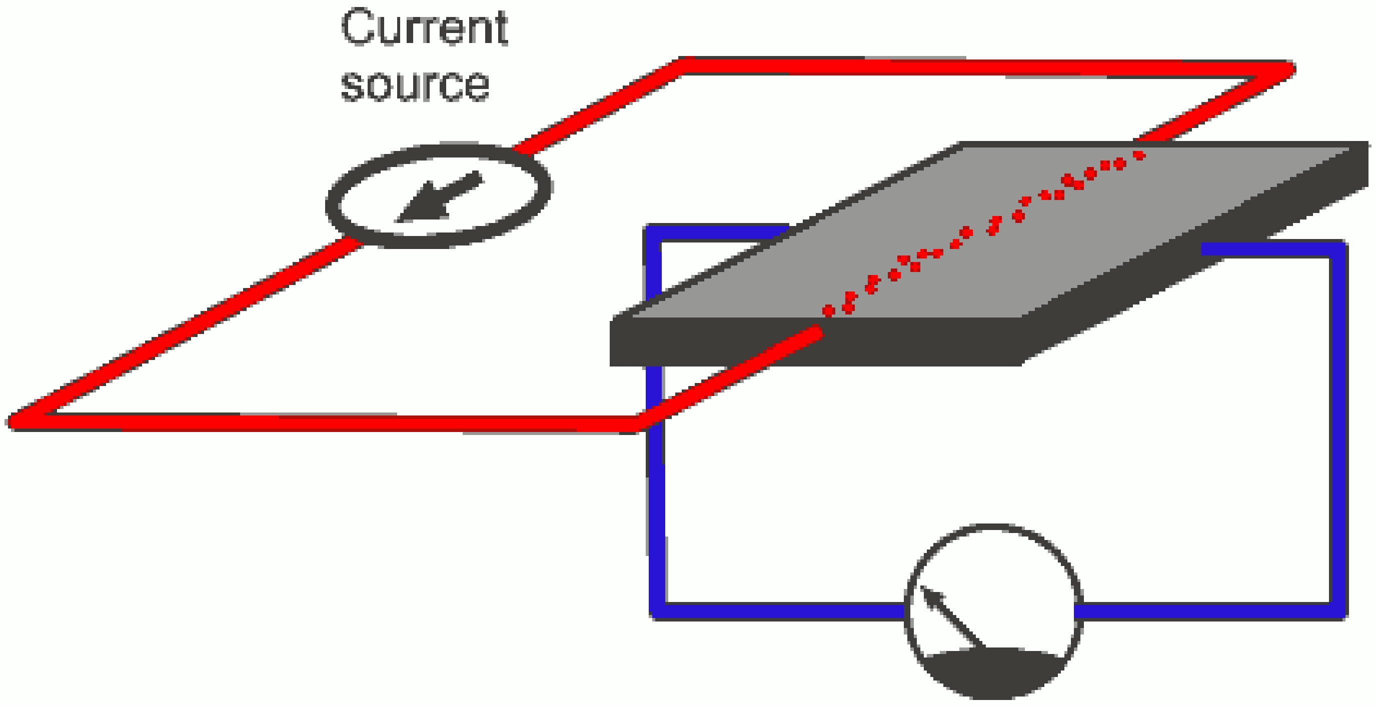
magnetic force





Hall Effect 霍尔效应

- A current flows through a conductor
- V_H is generated when applying B_z



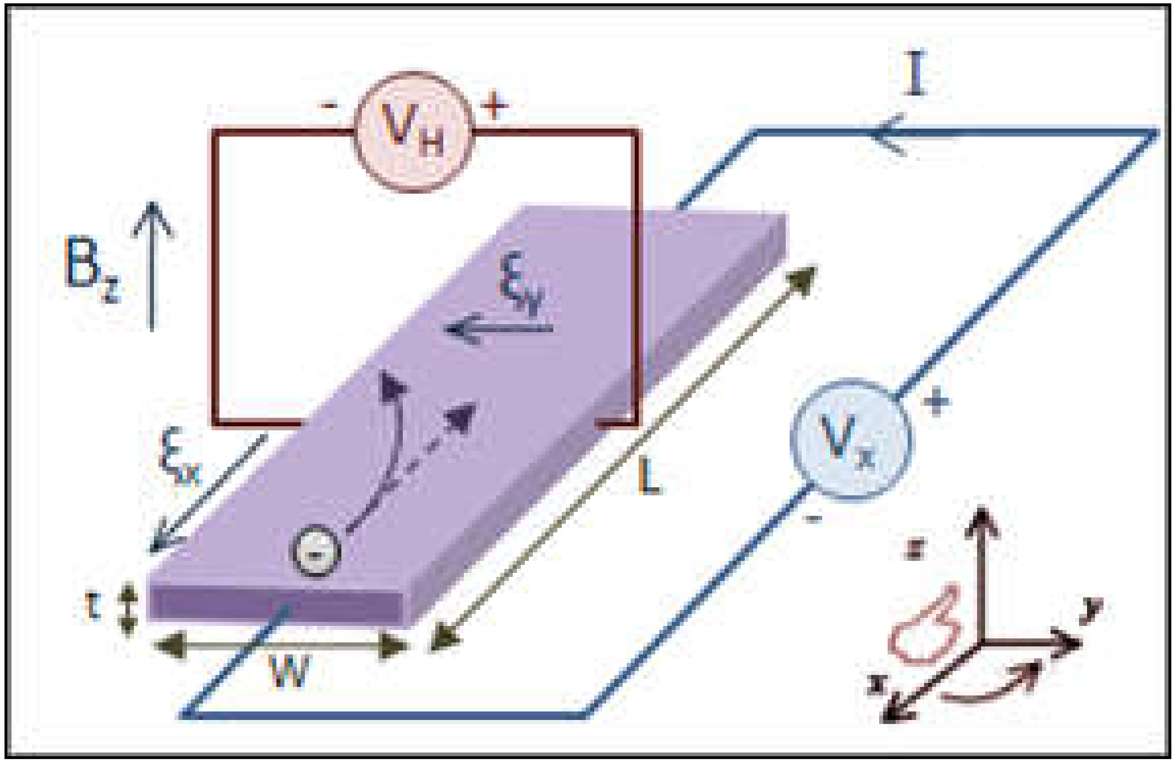
V_H - Hall voltage

Hall Effect 霍尔效应

- **A current flows through a conductor**
- **V_H is generated when applying B_z**

$$V_H = E_y \cdot w$$

$$E_y = R_H \cdot B_z \cdot j_x$$



R_H - Hall coefficient

By definition:
positive charge: $R_H > 0$
negative charge: $R_H < 0$

https://www.tf.uni-kiel.de/matwis/amat/mw2_ge/kap_2/backbone/r2_1_3.html

Quantum Mechanics

- **Wave-Particle Duality 波粒二象性**
- **De Broglie Wave 德布罗意波 / 物质波**

wavelength 波长

$$\boxed{\lambda = \frac{h}{p}}$$

wavenumber 波数
wavevector 波矢

$$\boxed{k = \frac{2\pi}{\lambda}}$$

momentum 动量

$$\boxed{p = mv = \hbar k}$$

energy 能量

$$\boxed{E = \frac{1}{2}mv^2 = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}}$$

$$\boxed{\hbar = \frac{h}{2\pi}}$$

Quantum Mechanics

- **Wave function for electrons** $\boxed{\psi(\mathbf{r},t)}$

$$\boxed{\left|\psi\right|^{2}=\psi^{*}\cdot\psi}$$

probability at (r, *t*)

$$\boxed{\psi(\mathbf{r},t)=\psi(\mathbf{r})\cdot\xi(t)}$$

- **Schrodinger Equation**

$$\boxed{\hat{H}\psi(\mathbf{r},t)=E\psi(\mathbf{r},t)}$$

Quantum Mechanics

- **Schrodinger Equation (time dependent)**

$$\boxed{-i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r},t)=E\psi(\mathbf{r},t)} \rightarrow \boxed{\xi(t)=\exp\left(-i\frac{E}{\hbar}t\right)}$$

$$\boxed{\hbar=\frac{h}{2\pi}}$$

- **Schrodinger Equation (time independent)**

$$\boxed{-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r},t)+V(\mathbf{r})\cdot\psi(\mathbf{r},t)=E\psi(\mathbf{r},t)}$$

$$\rightarrow \boxed{-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r})+V(\mathbf{r})\cdot\psi(\mathbf{r})=E\psi(\mathbf{r})}$$

Quantum Mechanics

- **Free electrons**

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r})+V(\mathbf{r})\cdot\psi(\mathbf{r})=E\psi(\mathbf{r})$$

free electron

$$V(\mathbf{r})=0$$

$$\rightarrow \quad \nabla^2\psi(\mathbf{r})=-k^2\psi(\mathbf{r})$$

$$k^2=\frac{2mE}{\hbar^2}$$

$$\rightarrow \quad \psi(\mathbf{r})=\sum_{\mathbf{k}}A_{\mathbf{k}}\exp(i\mathbf{k}\cdot\mathbf{r})$$

$$\int_V\psi^*\cdot\psi d\mathbf{r}=1$$

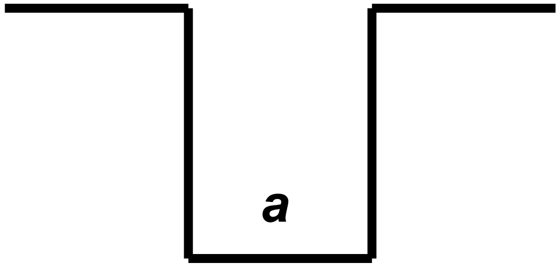
probability = 1

Quantum Mechanics

- **Electron in a box (1D infinite well)**

$$\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x)+V(x)\cdot\psi(x)=E\psi(x)}$$

$$\boxed{k^2=\frac{2mE}{\hbar^2}}$$



$$\begin{cases} V(x)=+\infty,\ \text{when } x<0 \\ V(x)=0,\ \text{when } 0<x<a \\ V(x)=+\infty,\ \text{when } x>a \end{cases}$$

for 0 < *x* < *a*

$$\boxed{\psi(x)=A\exp(ikx)+B\exp(-ikx)}$$

and

$$\boxed{\psi(x=0)=\psi(x=a)=0}$$

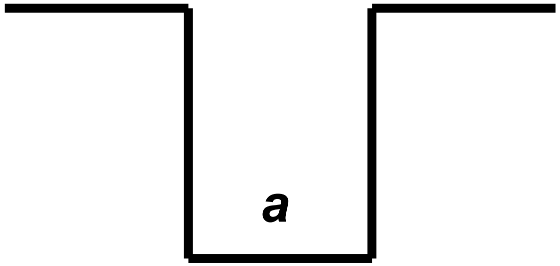
$$\boxed{\int_0^a \psi(x)dx=1}$$

Quantum Mechanics

- **Electron in a box (1D infinite well)**

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

$$k^2=\frac{2mE}{\hbar^2}$$



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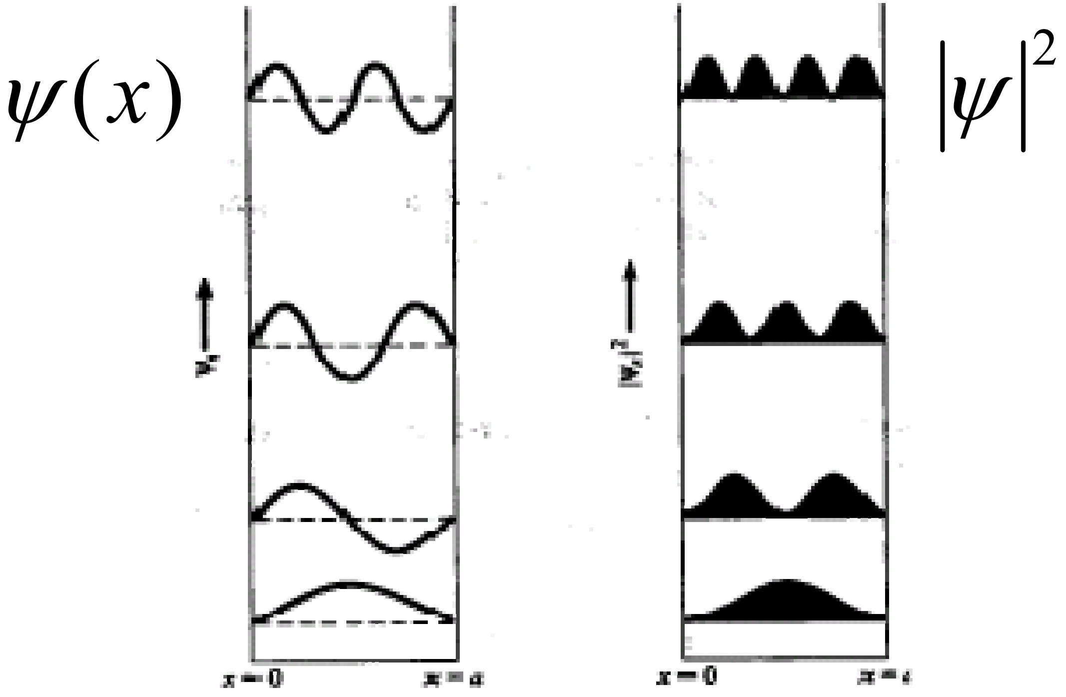
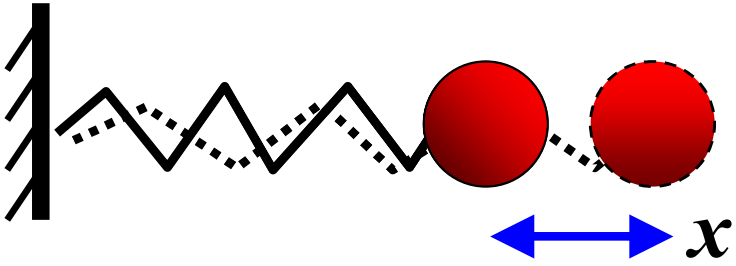


Quantum Mechanics

- **1D Harmonic Oscillator**

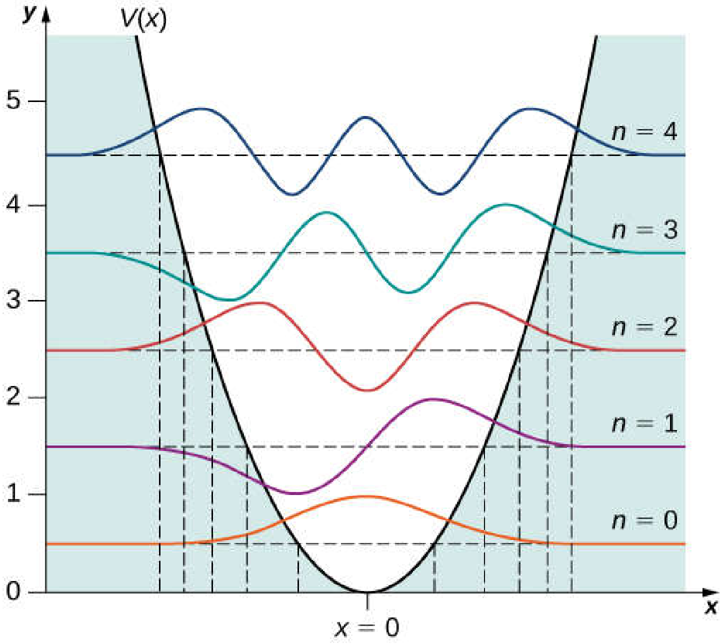


$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x)+V(x)\cdot\psi(x)=E\psi(x)$$

$$V(x)=\frac{1}{2}Kx^2=\frac{1}{2}m\omega^2x^2$$

$$\omega=\sqrt{\frac{K}{m}}$$

$$\rightarrow \quad E_n=\left(\frac{1}{2}+n\right)\hbar\omega \qquad n=0,1,2,\ldots$$



$$\psi_n(x)=e^{-\beta x^2/2}\cdot H_n(x)$$

$$\beta=\frac{\sqrt{Km}}{\hbar}$$

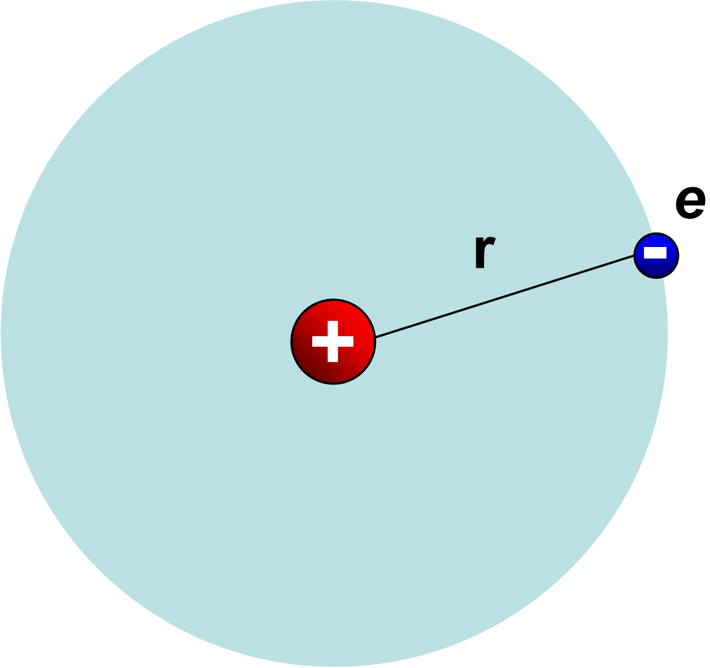
$H_n(x)$

Hermite polynomial

Quantum Mechanics

- **Hydrogen atom**

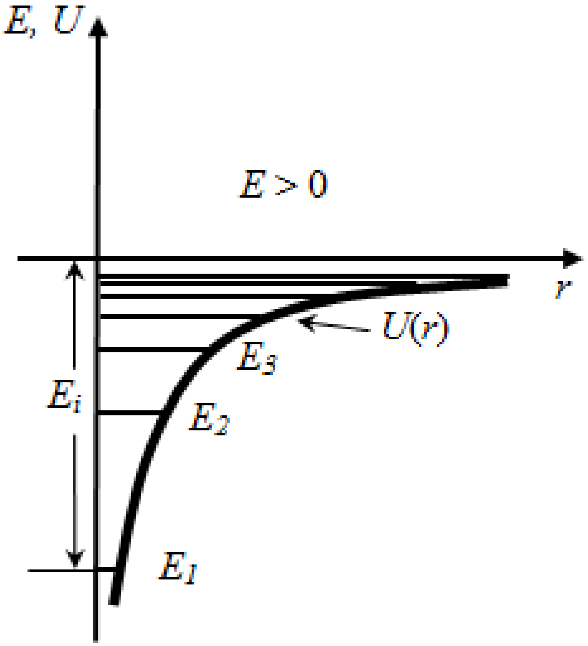
$$V(\mathbf{r}) = -\frac{e^2}{4\pi\varepsilon_0}\frac{1}{\mathbf{r}}$$



Quantum Mechanics

- **Hydrogen atom**

$$V(\mathbf{r}) = -\frac{e^2}{4\pi\varepsilon_0}\frac{1}{\mathbf{r}}$$



$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) + V(\mathbf{r})\cdot\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

$$\rightarrow \quad \psi(r,\theta,\varphi) = R_{nl}(r)\cdot Y_{lm}(\theta,\varphi)$$

$$E_n = -\frac{me^4}{8\varepsilon_0^2 h^2 n^2} = -\frac{13.6\,\mathrm{eV}}{n^2}$$

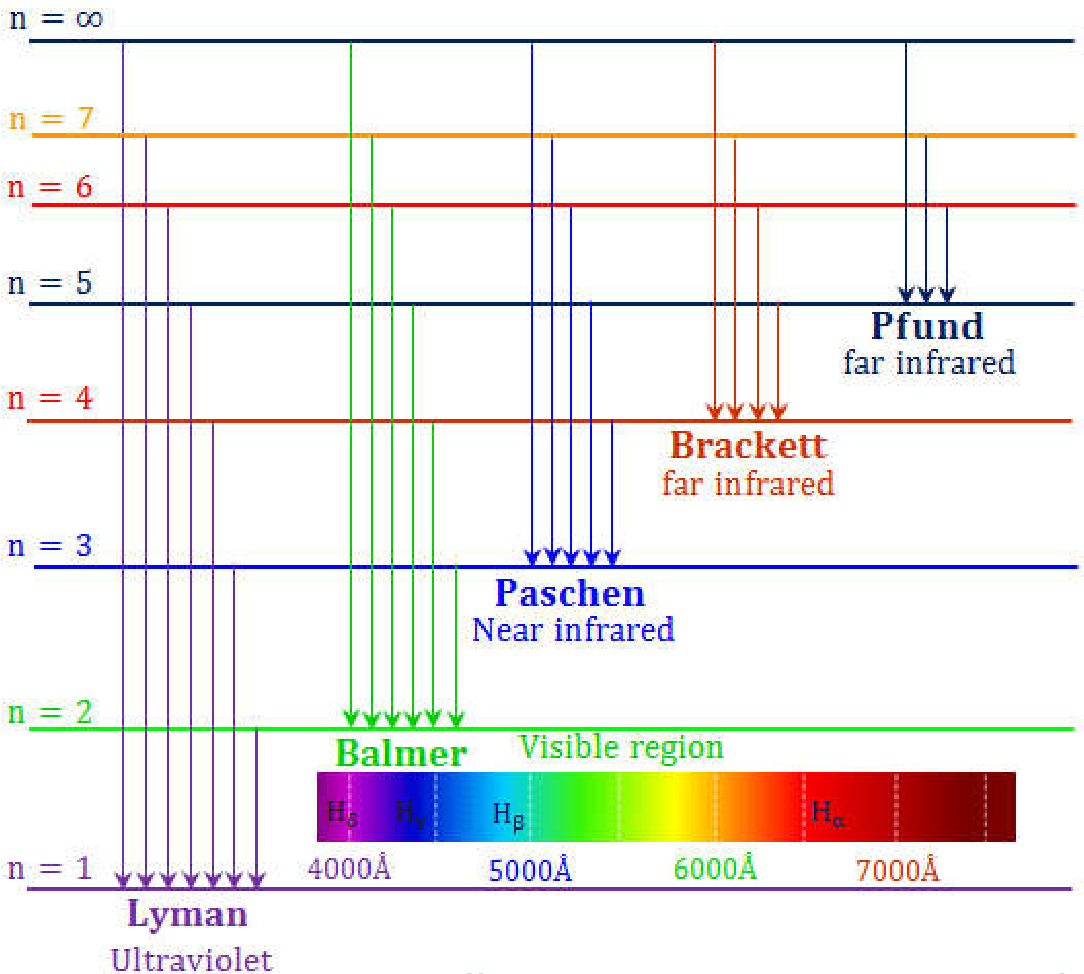
***n*, *l*, *m* - quantum numbers**

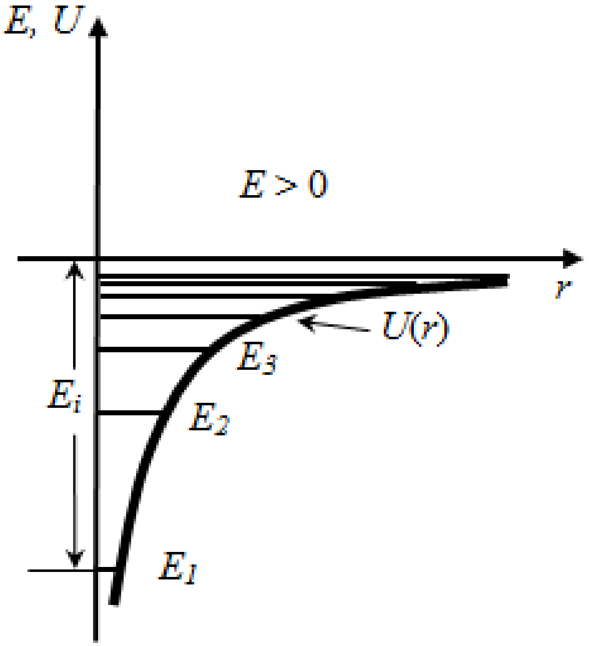
m_S - spin (+1/2, -1/2)

Quantum Mechanics

- **Hydrogen atom**

$$E_n = -\frac{13.6\,\mathrm{eV}}{n^2}$$





Emissions of atoms have discrete energy lines

https://www.priyamstudycentre.com/2019/02/hydrogen-spectrum.html

Atoms with Many Electrons

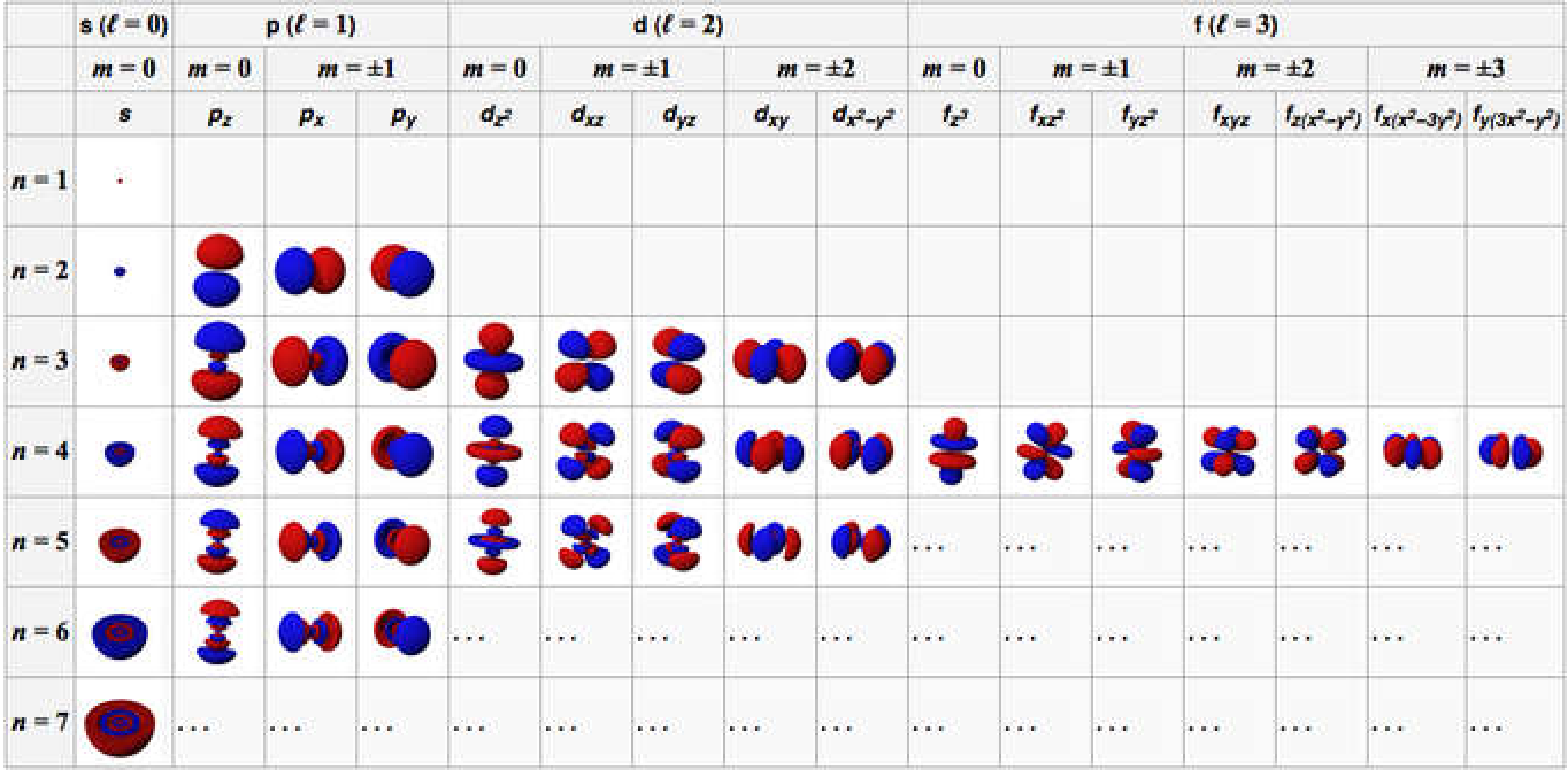
- **Quantum Numbers n, l, m, m_s**
  - Principal: n = 1, 2, 3, 4, ...
  - Angular momentum: l = 0, 1, 2, 3, ... (n–1)
  - Magnetic: m = $-l$, ..., –1, 0, +1, ... $+l$
  - Spin: m_s = +1/2, –1/2

$$\boxed{\psi(r,\theta,\varphi) = R_{nl}(r)\cdot Y_{lm}(\theta,\varphi)}$$

https://courses.lumenlearning.com/introchem/chapter/quantum-numbers/

Atoms with Many Electrons

- **Quantum Numbers *n, l, m, m_s***



	s ($\ell = 0$)	p ($\ell = 1$)			d ($\ell = 2$)					f ($\ell = 3$)						
	$m = 0$	$m = 0$	$m = \pm 1$		$m = 0$	$m = \pm 1$		$m = \pm 2$		$m = 0$	$m = \pm 1$		$m = \pm 2$		$m = \pm 3$	
	s	p_z	p_x	p_y	d_{z^2}	d_{xz}	d_{yz}	d_{xy}	$d_{x^2-y^2}$	f_{z^3}	f_{xz^2}	f_{yz^2}	f_{xyz}	$f_{z(x^2-y^2)}$	$f_{x(x^2-3y^2)}$	$f_{y(3x^2-y^2)}$
$n = 1$																
$n = 2$																
$n = 3$																
$n = 4$																
$n = 5$										...	...	...	...	...	...	...
$n = 6$					...	...	...	...	...	...	...	...	...	...	...	...
$n = 7$		...	...	...	...	...	...	...	...	...	...	...	...	...	...	...

https://courses.lumenlearning.com/introchem/chapter/quantum-numbers/

Quantum Mechanics

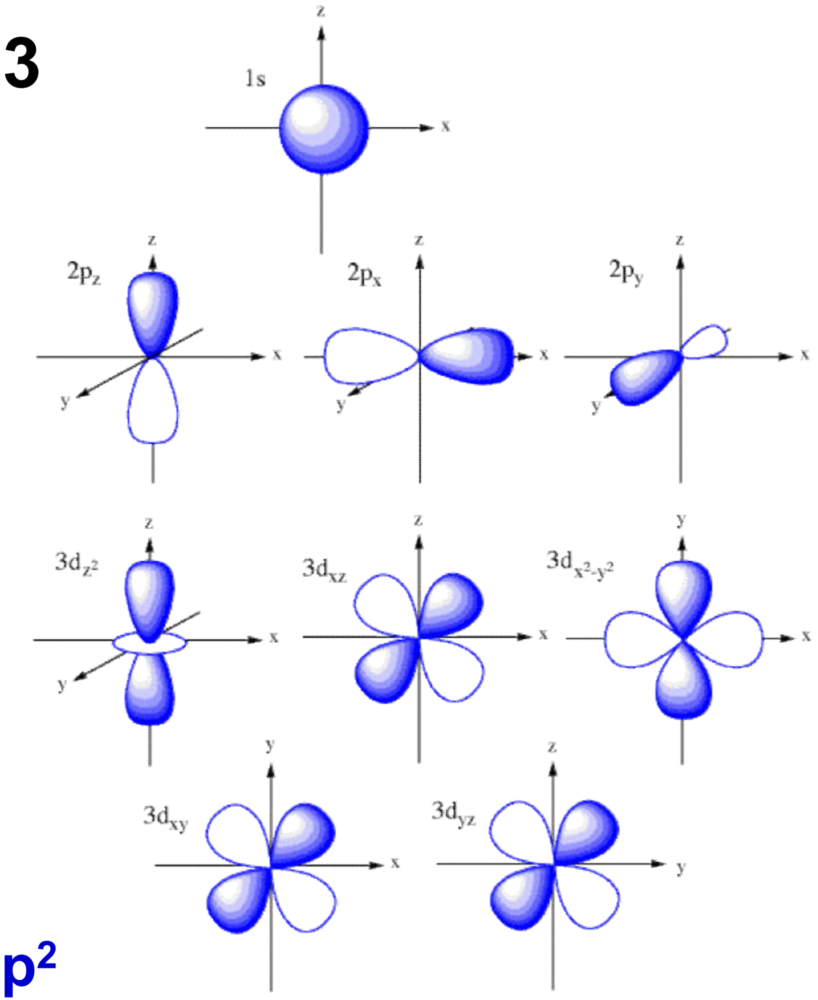
- Angular momentum: *l* = 0, 1, 2, 3
- Atomic orbitals: s p d f

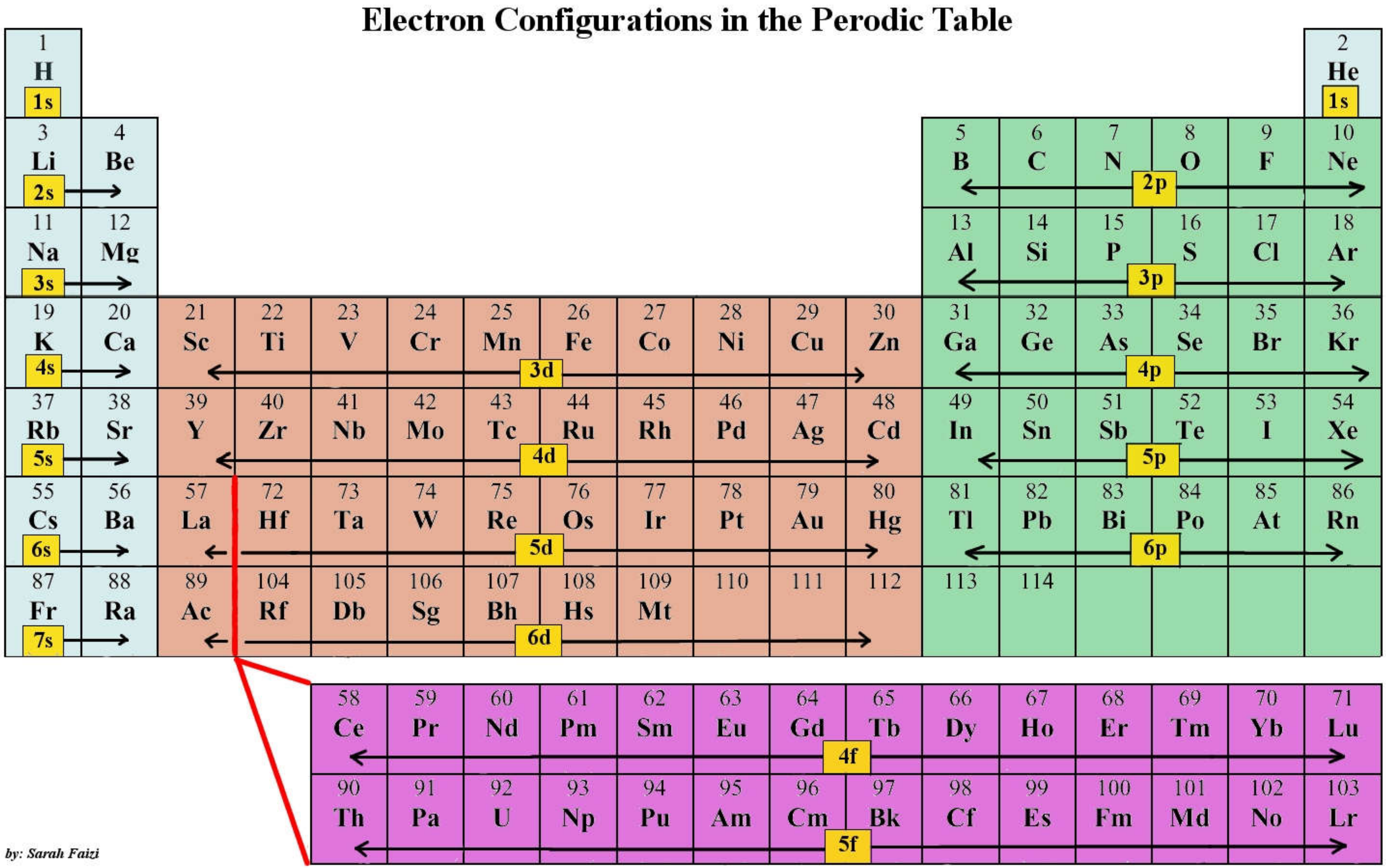
- Examples

Hydrogen (H)	$1s^1$
Helium (He)	$1s^2$
Lithium (Li)	$[1s^2]\ 2s^1$
Carbon (C)	$[1s^2]\ 2s^2\ 2p^2$
Neon (Ne)	$[1s^2]\ 2s^2\ 2p^6$
Sodium (Na)	$[1s^2\ 2s^2\ 2p^6]\ 3s^1$
Silicon (Si)	$\underbrace{[1s^2\ 2s^2\ 2p^6]}\ \underbrace{3s^2\ 3p^2}$

core electrons

valence electrons





Electron Configurations in the Perodic Table

1 H 1s																	2 He 1s
3 Li 2s	4 Be											5 B	6 C	7 N	8 O 2p	9 F	10 Ne
11 Na 3s	12 Mg											13 Al	14 Si	15 P 3p	16 S	17 Cl	18 Ar
19 K 4s	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe 3d	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As 4p	34 Se	35 Br	36 Kr
37 Rb 5s	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru 4d	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te 5p	53 I	54 Xe
55 Cs 6s	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os 5d	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po 6p	85 At	86 Rn
87 Fr 7s	88 Ra	89 Ac	104 Rf	105 Db	106 Sg	107 Bh 6d	108 Hs	109 Mt	110	111	112	113	114				
				58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb 4f	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
				90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk 5f	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

by: Sarah Faizi

Statistical Mechanics

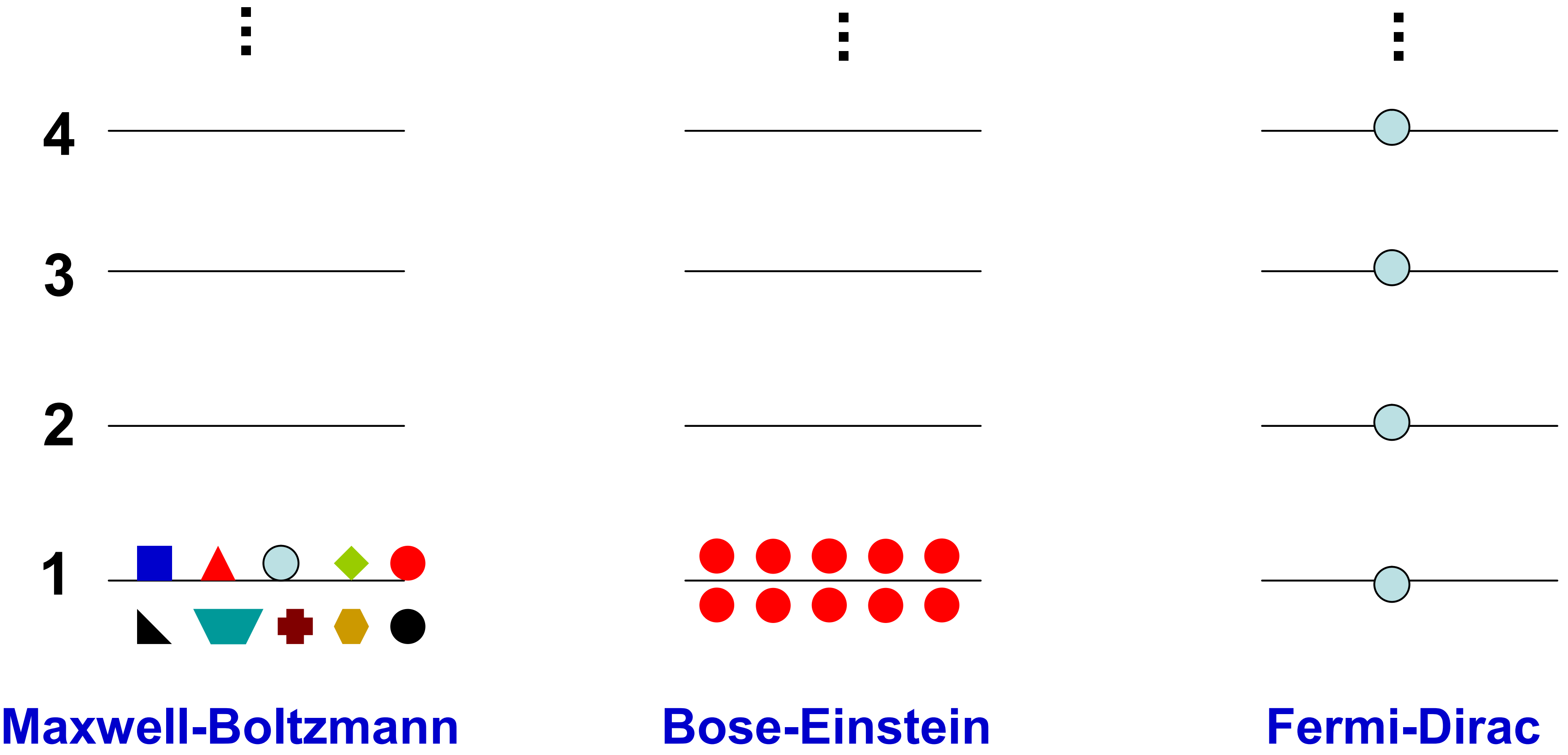
- **Maxwell–Boltzmann Distribution 玻尔兹曼分布**
  - distinguishable, non-interaction particles: ideal gas, ...

- **Bose–Einstein Distribution 玻色-爱因斯坦分布**
  - indistinguishable particles
  - Bosons: photons, phonons, ...
  - integer spin

- **Fermi–Dirac Distribution 费米-狄拉克分布**
  - indistinguishable particles
  - Fermions: electrons, ...
  - half-integer spin
  - Pauli exclusion principle (泡利不相容原理)

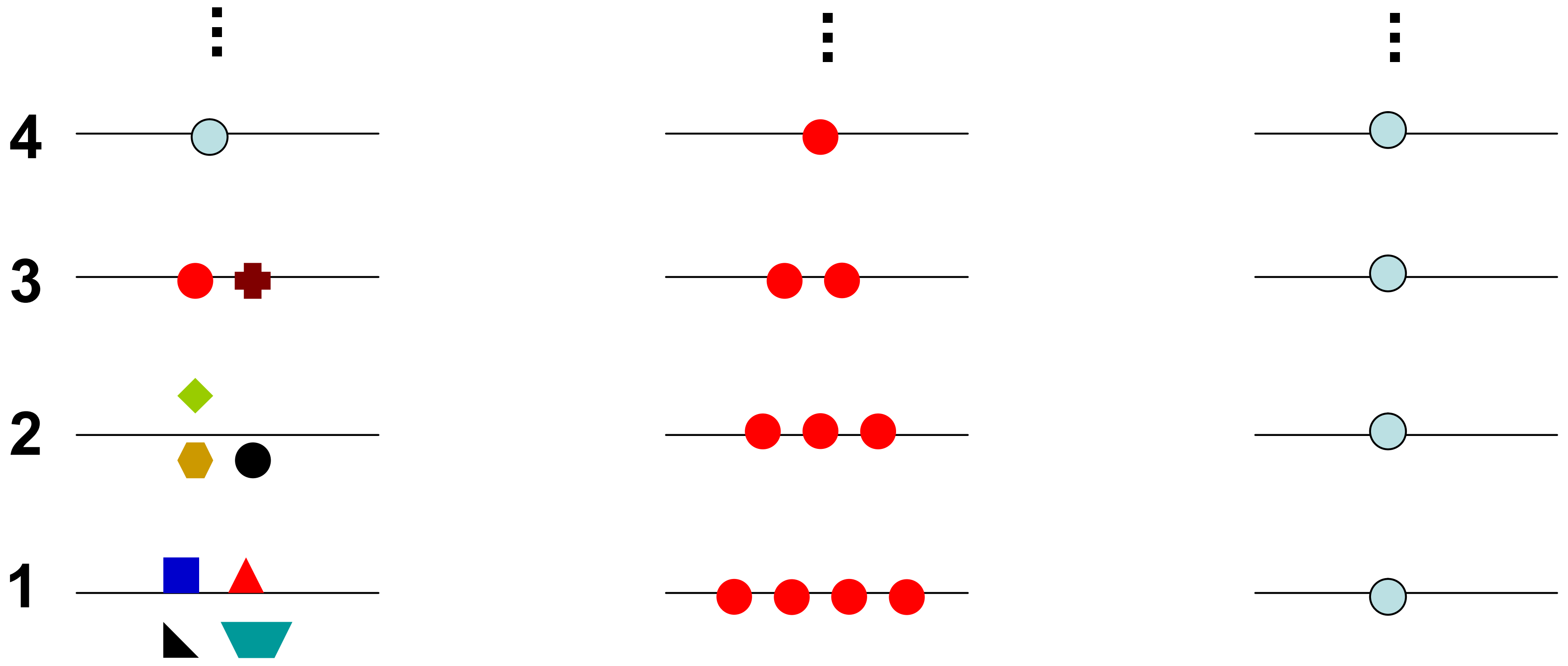
Statistical Mechanics

- At *T* = 0 K



Statistical Mechanics

- **At T > 0 K**



Maxwell-Boltzmann **Bose-Einstein** **Fermi-Dirac**

Statistical Mechanics

- **Fermi–Dirac Distribution**
  - Fermions: electrons, ...

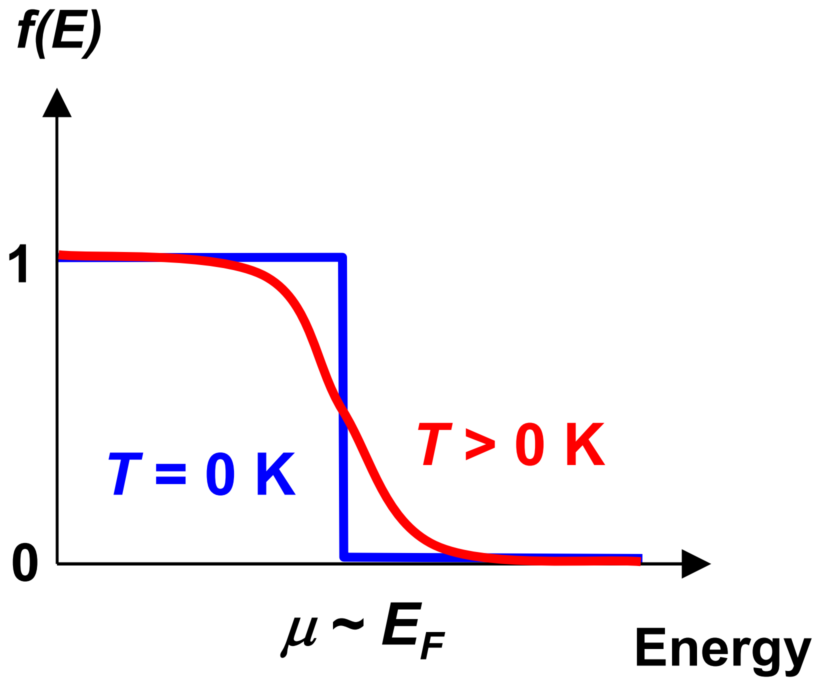
$$f(E) = \frac{1}{e^{(E-\mu)/k_B T} + 1}$$

$f(E)$ - probability that an energy state E is occupied

μ - chemical potential

E_F - Fermi energy

$\mu = E_F$ when $T = 0$ K

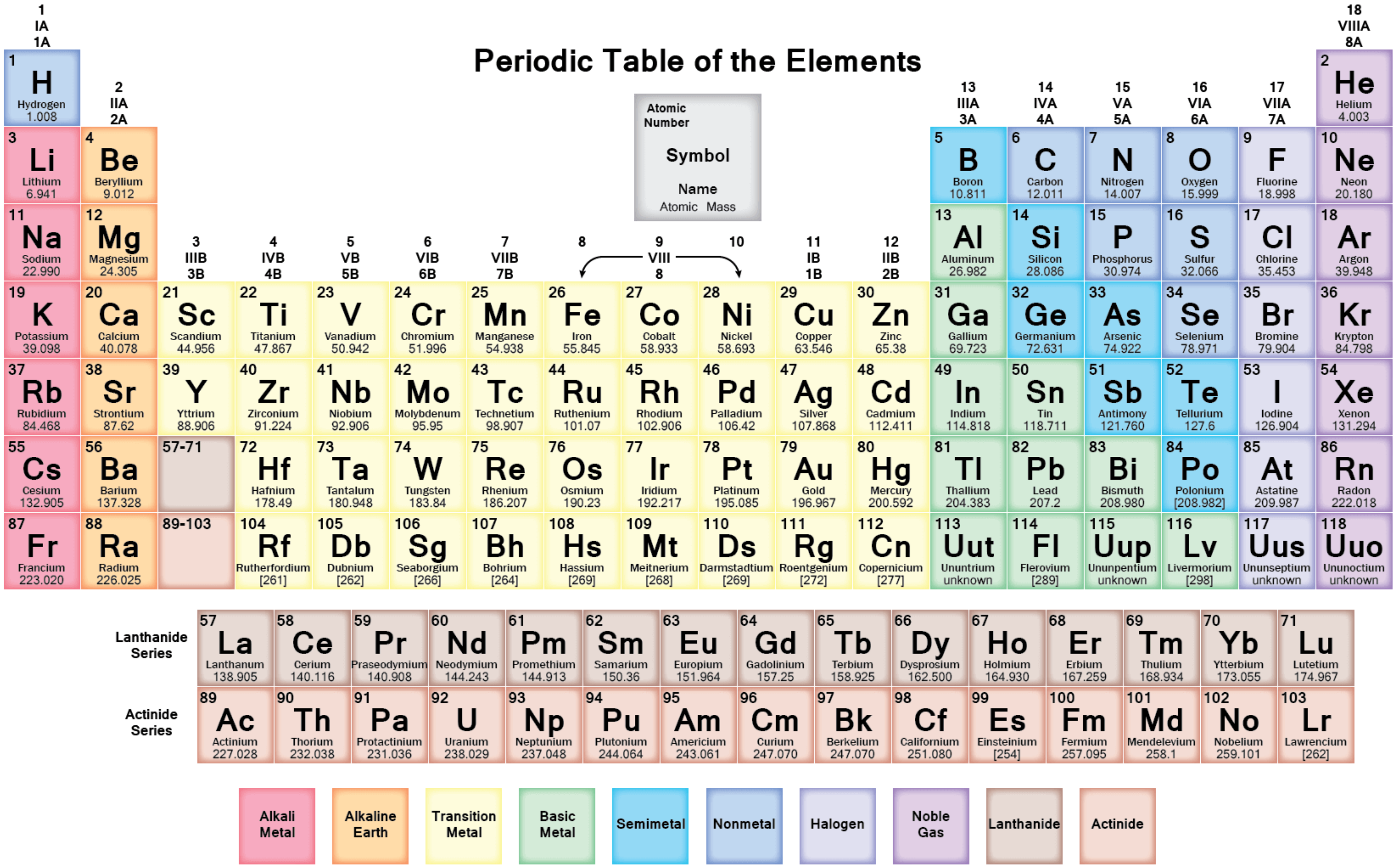


At $T = 0$ K

$f(E) = 1$ for $E < \mu$

$f(E) = 0$ for $E > \mu$

Chemistry



Periodic Table of the Elements

Atomic Number
Symbol
Name
Atomic Mass

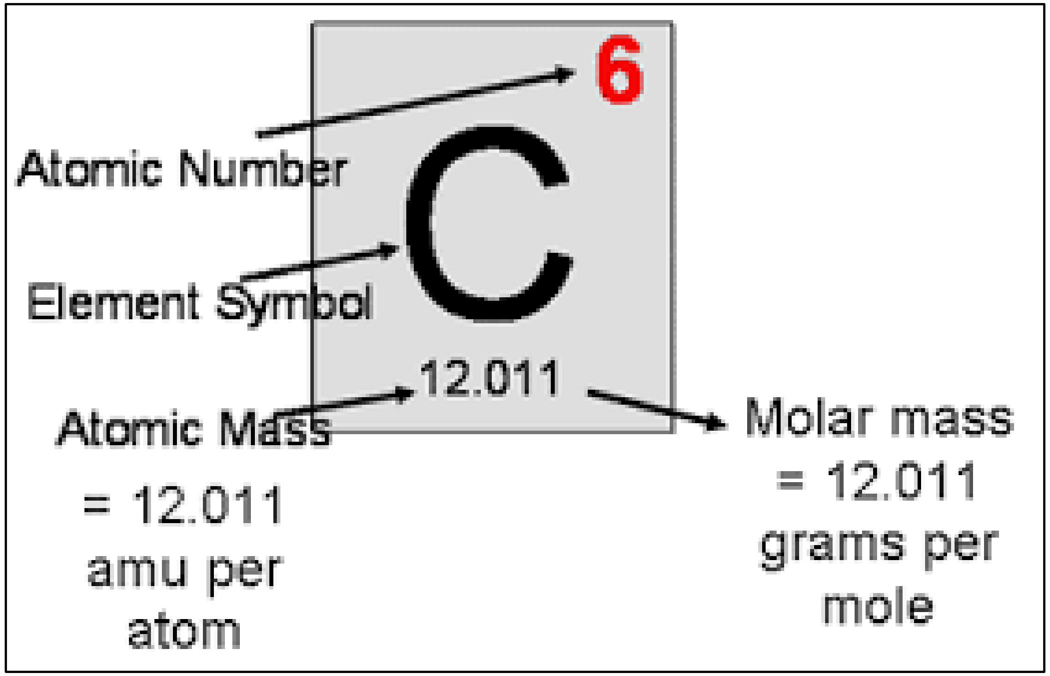
1 IA 1A	2 IIA 2A	3 IIIB 3B	4 IVB 4B	5 VB 5B	6 VIB 6B	7 VIIB 7B	8	9 VIII 8	10	11 IB 1B	12 IIB 2B	13 IIIA 3A	14 IVA 4A	15 VA 5A	16 VIA 6A	17 VIIA 7A	18 VIIIA 8A
1 H Hydrogen 1.008																	2 He Helium 4.003
3 Li Lithium 6.941	4 Be Beryllium 9.012											5 B Boron 10.811	6 C Carbon 12.011	7 N Nitrogen 14.007	8 O Oxygen 15.999	9 F Fluorine 18.998	10 Ne Neon 20.180
11 Na Sodium 22.990	12 Mg Magnesium 24.305											13 Al Aluminum 26.982	14 Si Silicon 28.086	15 P Phosphorus 30.974	16 S Sulfur 32.066	17 Cl Chlorine 35.453	18 Ar Argon 39.948
19 K Potassium 39.098	20 Ca Calcium 40.078	21 Sc Scandium 44.956	22 Ti Titanium 47.867	23 V Vanadium 50.942	24 Cr Chromium 51.996	25 Mn Manganese 54.938	26 Fe Iron 55.845	27 Co Cobalt 58.933	28 Ni Nickel 58.693	29 Cu Copper 63.546	30 Zn Zinc 65.38	31 Ga Gallium 69.723	32 Ge Germanium 72.631	33 As Arsenic 74.922	34 Se Selenium 78.971	35 Br Bromine 79.904	36 Kr Krypton 84.798
37 Rb Rubidium 84.468	38 Sr Strontium 87.62	39 Y Yttrium 88.906	40 Zr Zirconium 91.224	41 Nb Niobium 92.906	42 Mo Molybdenum 95.95	43 Tc Technetium 98.907	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.906	46 Pd Palladium 106.42	47 Ag Silver 107.868	48 Cd Cadmium 112.411	49 In Indium 114.818	50 Sn Tin 118.711	51 Sb Antimony 121.760	52 Te Tellurium 127.6	53 I Iodine 126.904	54 Xe Xenon 131.294
55 Cs Cesium 132.905	56 Ba Barium 137.328	57-71	72 Hf Hafnium 178.49	73 Ta Tantalum 180.948	74 W Tungsten 183.84	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.217	78 Pt Platinum 195.085	79 Au Gold 196.967	80 Hg Mercury 200.592	81 Tl Thallium 204.383	82 Pb Lead 207.2	83 Bi Bismuth 208.980	84 Po Polonium [208.982]	85 At Astatine 209.987	86 Rn Radon 222.018
87 Fr Francium 223.020	88 Ra Radium 226.025	89-103	104 Rf Rutherfordium [261]	105 Db Dubnium [262]	106 Sg Seaborgium [266]	107 Bh Bohrium [264]	108 Hs Hassium [269]	109 Mt Meitnerium [268]	110 Ds Darmstadtium [269]	111 Rg Roentgenium [272]	112 Cn Copernicium [277]	113 Uut Ununtrium unknown	114 Fl Flerovium [289]	115 Uup Ununpentium unknown	116 Lv Livermorium [298]	117 Uus Ununseptium unknown	118 Uuo Ununoctium unknown

Lanthanide Series	57 La Lanthanum 138.905	58 Ce Cerium 140.116	59 Pr Praseodymium 140.908	60 Nd Neodymium 144.243	61 Pm Promethium 144.913	62 Sm Samarium 150.36	63 Eu Europium 151.964	64 Gd Gadolinium 157.25	65 Tb Terbium 158.925	66 Dy Dysprosium 162.500	67 Ho Holmium 164.930	68 Er Erbium 167.259	69 Tm Thulium 168.934	70 Yb Ytterbium 173.055	71 Lu Lutetium 174.967
Actinide Series	89 Ac Actinium 227.028	90 Th Thorium 232.038	91 Pa Protactinium 231.036	92 U Uranium 238.029	93 Np Neptunium 237.048	94 Pu Plutonium 244.064	95 Am Americium 243.061	96 Cm Curium 247.070	97 Bk Berkelium 247.070	98 Cf Californium 251.080	99 Es Einsteinium [254]	100 Fm Fermium 257.095	101 Md Mendelevium 258.1	102 No Nobelium 259.101	103 Lr Lawrencium [262]

Alkali Metal	Alkaline Earth	Transition Metal	Basic Metal	Semimetal	Nonmetal	Halogen	Noble Gas	Lanthanide	Actinide

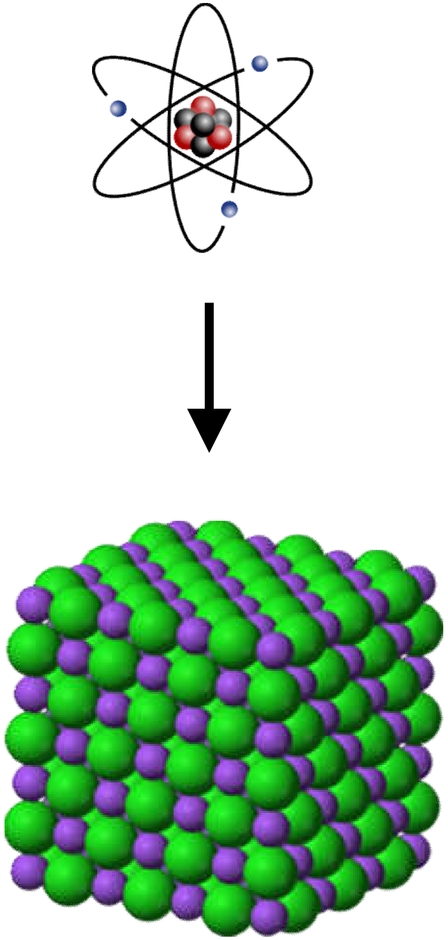
Chemistry

- **Periodic Table**
- **Atomic number**
- **Mass number**
  - amu / atom
  - g / mol
- **Avogadro's number N_A**
  - 1 mol = $6.022 * 10^{23}$



Chemical Bonding 化学键

- Solids are formed by chemical bonding between atoms
  - Metallic Bonding 金属键
  - Ionic Bonding 离子键
  - Covalent Bonding 共价键
  - Van der Waals Bonding 范德华键
  - Hydrogen Bonding 氢键
  - ...

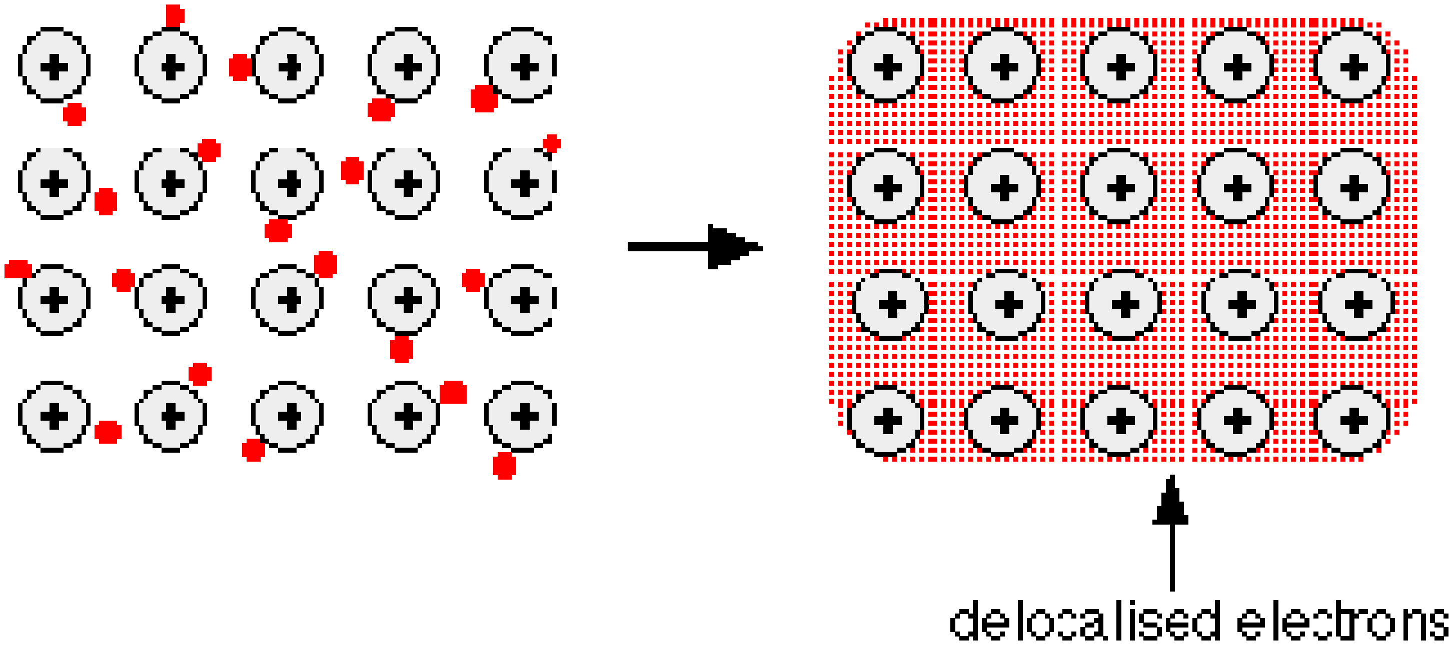


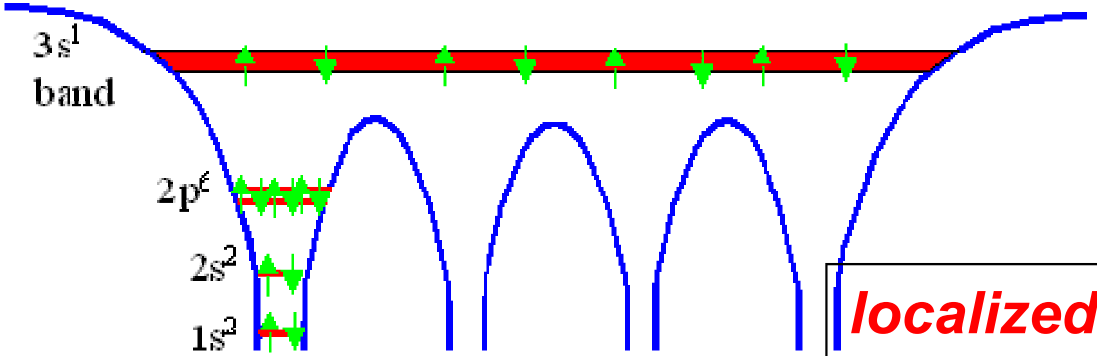
- Valence electrons form bonds
  - Silicon (Si) $[1s^2\ 2s^2\ 2p^6]\ \underline{3s^2\ 3p^2}$

https://www.chemguide.co.uk/atoms/bondingmenu.html

Metallic Bonding 金属键

- **Positive metal ions in a sea of delocalised electrons**





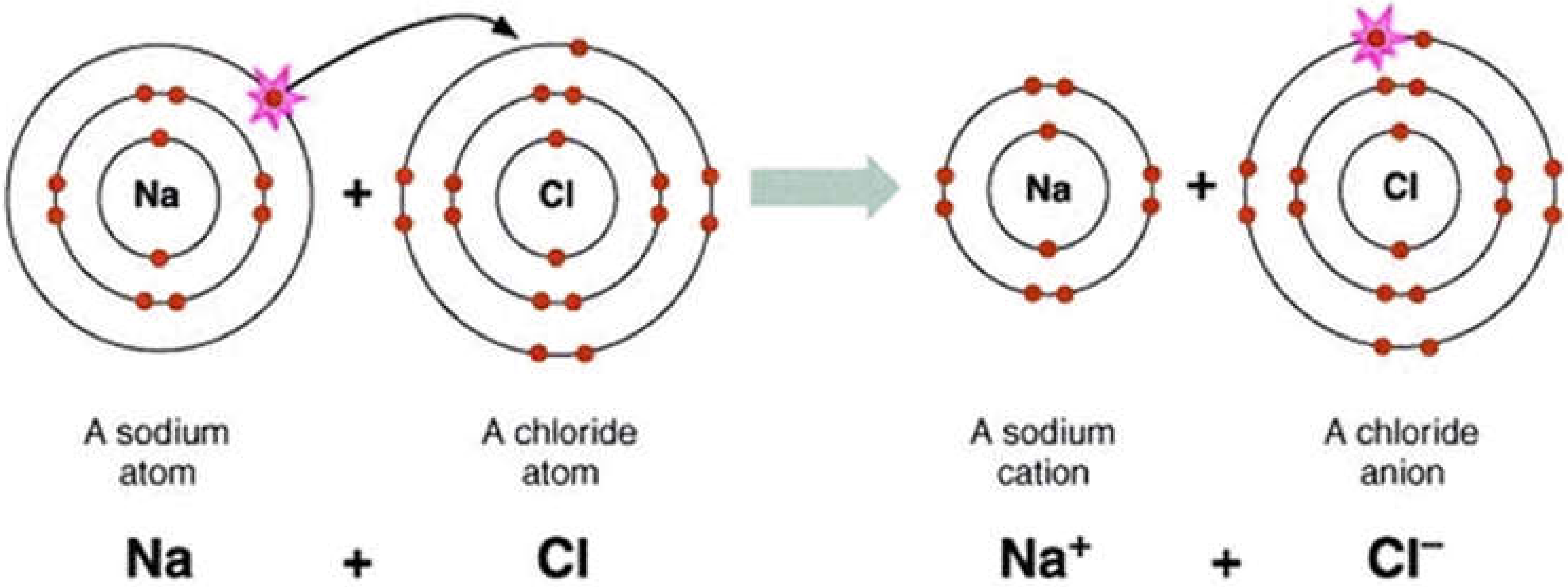
Sodium (Na) $[1s^2\ 2s^2\ 2p^6]\ 3s^1$

localized electron (core electron)

'delocalized' electron (free electron)

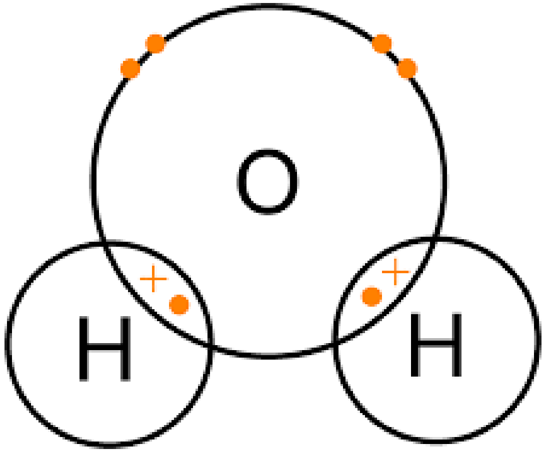
Ionic Bonding 离子键

- **NaCl**
    - Na loses an electron → Na^+ (cation)
    - Cl gains an electron → Cl^- (anion)
    - Cations and anions are held by electrostatic attractions

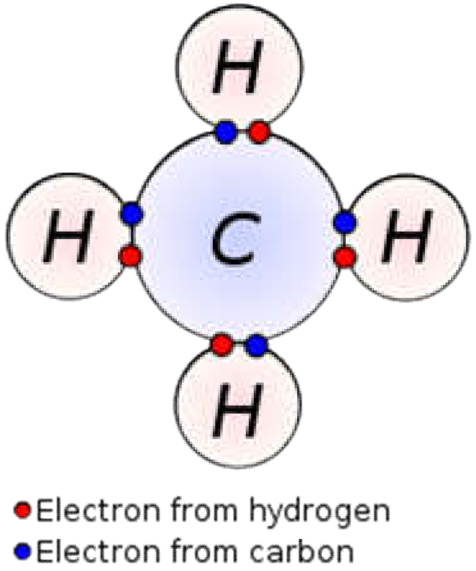


Covalent Bonding 共价键

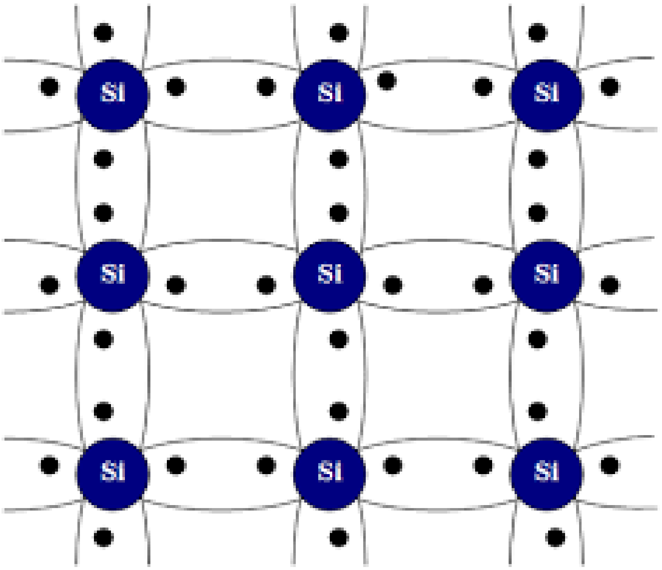
- Electron pairs are shared between atoms



H_2O



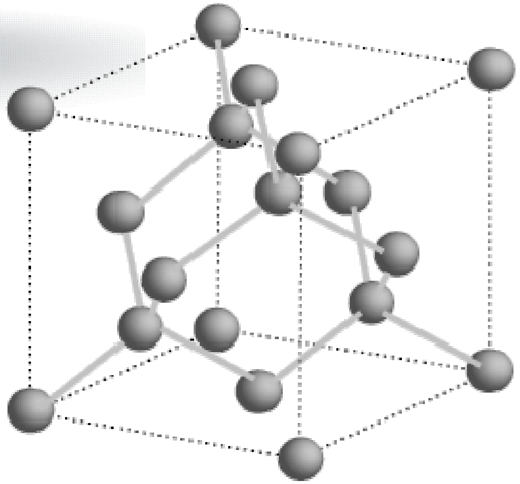
CH_4



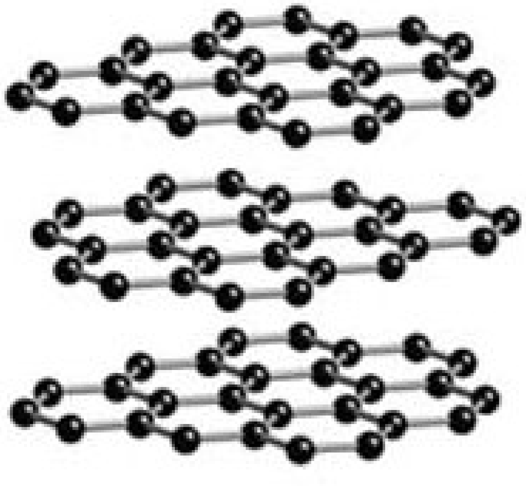
Silicon

Example: Carbon

- Diamond is the hardest material and an insulator
  - all the 4 valence electrons form covalent bonds
- Graphite is the softest solid and a conductor
  - atoms in each plane form covalent bonds (3 electrons)
  - There is one free electron
  - stacking layers form metallic bonds

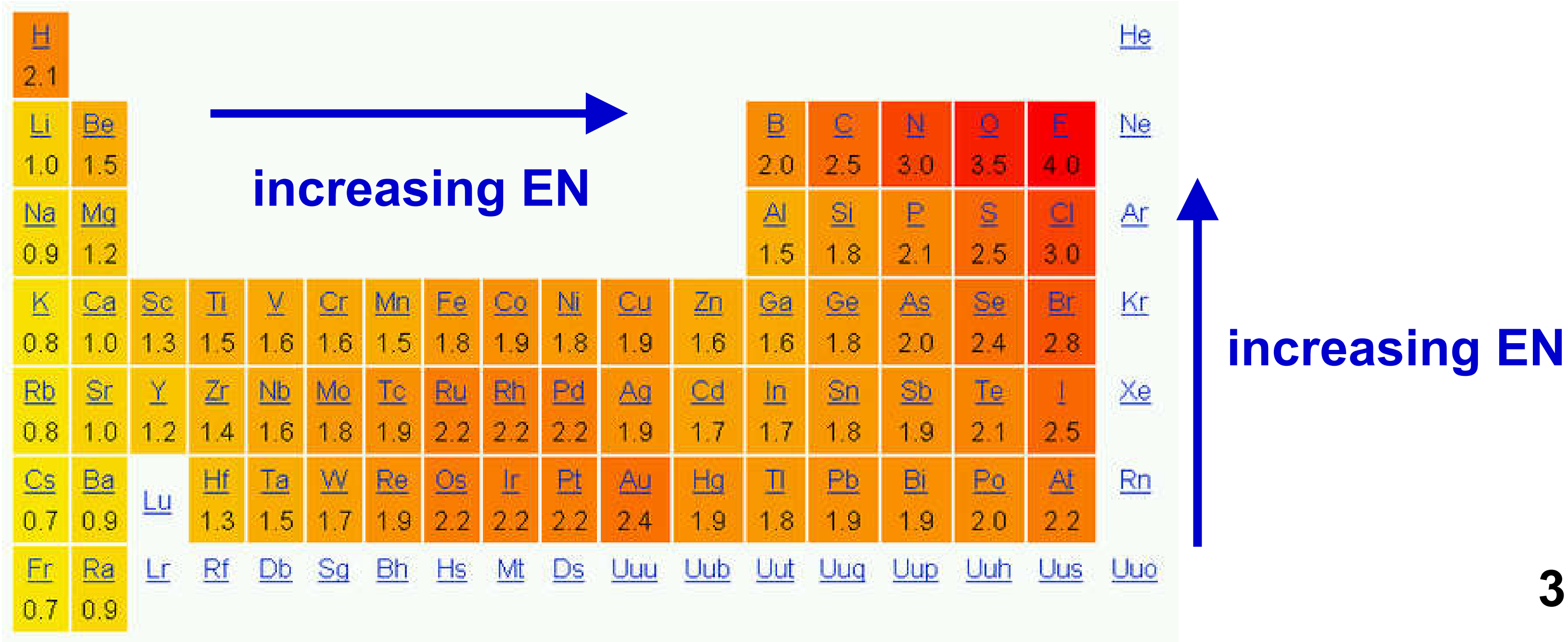
diamond
金刚石




graphite
石墨

Electronegativity (EN) 电负性

- **Tendency of an atom to attract a bonding pair of electrons**
  - EN(Li) = 1.0   EN(F) = 4.0
- **A-B bond usually has mixed bonding properties**
  - similar EN → more covalent bonding
  - different EN → more ionic bonding

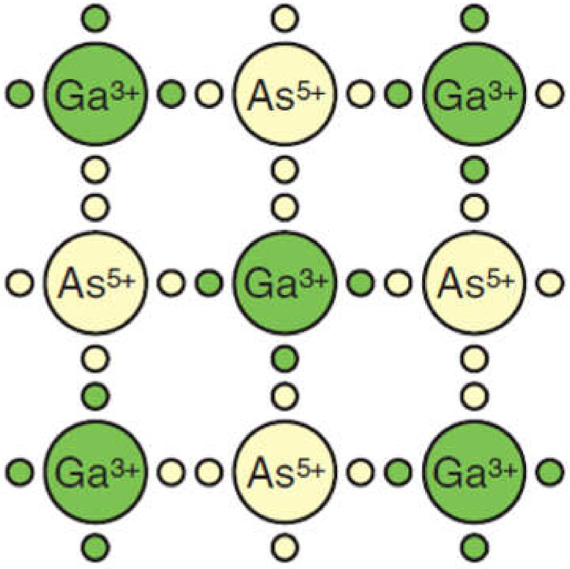


H 2.1																	He
Li 1.0	Be 1.5											B 2.0	C 2.5	N 3.0	O 3.5	F 4.0	Ne
Na 0.9	Mg 1.2											Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0	Ar
K 0.8	Ca 1.0	Sc 1.3	Ti 1.5	V 1.6	Cr 1.6	Mn 1.5	Fe 1.8	Co 1.9	Ni 1.8	Cu 1.9	Zn 1.6	Ga 1.6	Ge 1.8	As 2.0	Se 2.4	Br 2.8	Kr
Rb 0.8	Sr 1.0	Y 1.2	Zr 1.4	Nb 1.6	Mo 1.8	Tc 1.9	Ru 2.2	Rh 2.2	Pd 2.2	Ag 1.9	Cd 1.7	In 1.7	Sn 1.8	Sb 1.9	Te 2.1	I 2.5	Xe
Cs 0.7	Ba 0.9	Lu	Hf 1.3	Ta 1.5	W 1.7	Re 1.9	Os 2.2	Ir 2.2	Pt 2.2	Au 2.4	Hg 1.9	Tl 1.8	Pb 1.9	Bi 1.9	Po 2.0	At 2.2	Rn
Fr 0.7	Ra 0.9	Lr	Rf	Db	Sg	Bh	Hs	Mt	Ds	Uuu	Uub	Uut	Uuq	Uup	Uuh	Uus	Uuo

Electronegativity (EN) 电负性

- NaCl has pure ionic bonding
- Silicon has pure covalent bonding

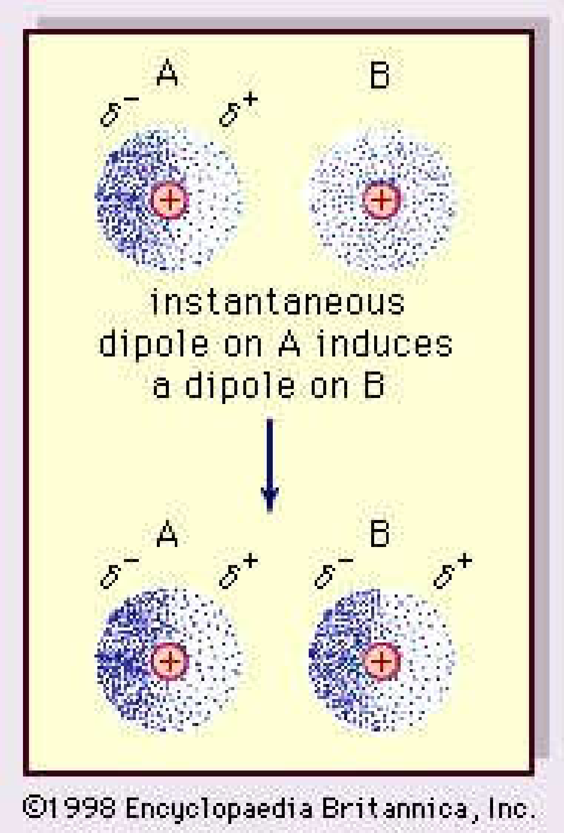
- Solids like GaAs and ZnSe have mixed ionic and covalent bonding



Van der Waals Bonding 范德华键

- **Attraction energy between neutral molecules / atoms**

$$\boxed{U(r) \propto -\frac{1}{r^6}}$$



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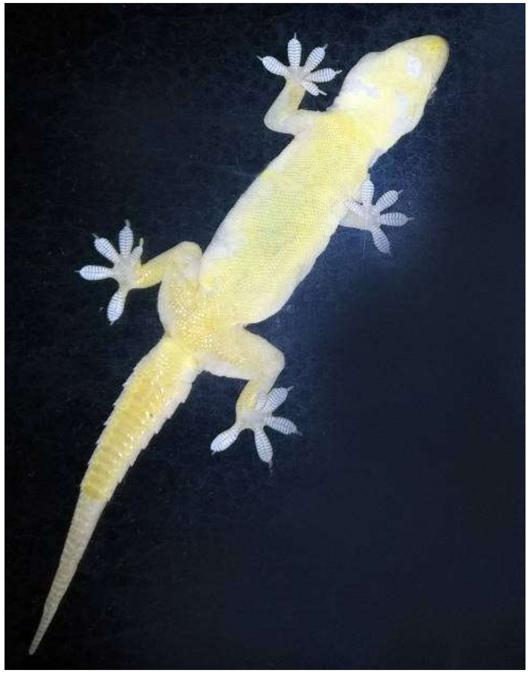
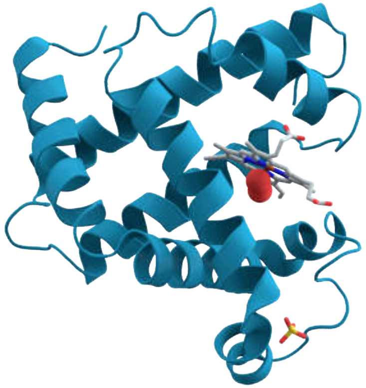


gecko 壁虎

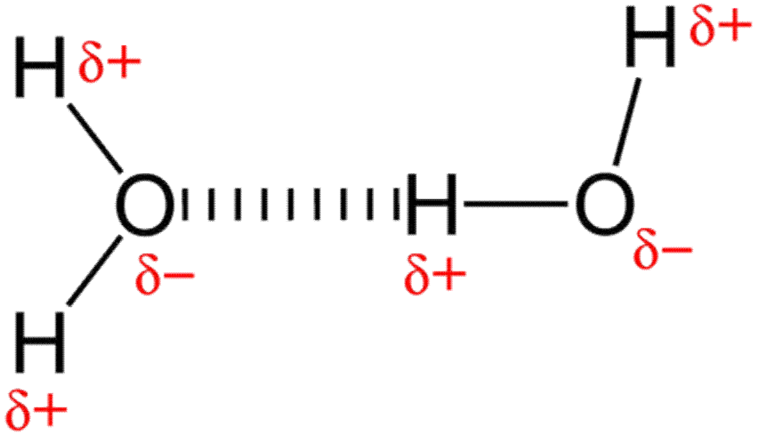
tape



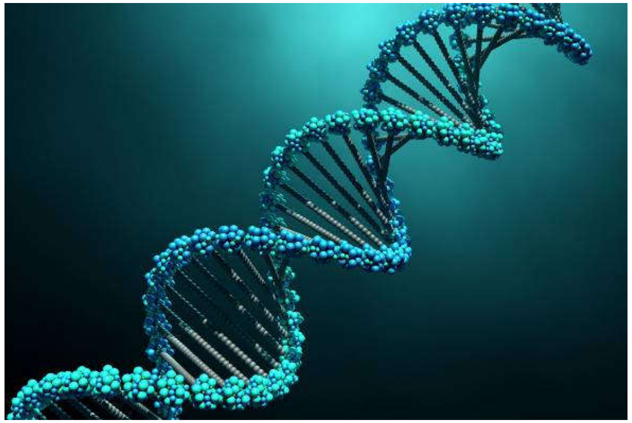
protein

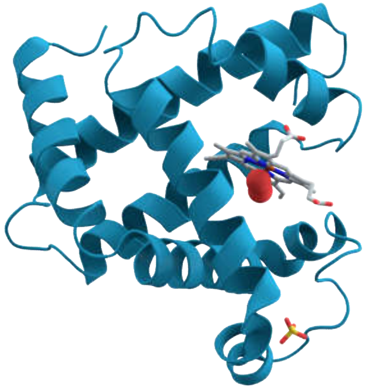
Hydrogen Bonding 氢键

- A special Van der Waals bond
  - generated by hydrogen




water


DNA


protein

Further Reading

- Quantum Mechanics
  - Physical Chemistry by Mortimer, Chap. 14-16
- Atoms and Chemical Bonding
  - Chemistry: The Central Science, Chap. 6, 8
  - https://ocw.mit.edu/courses/earth-atmospheric-and-planetary-sciences/12-108-structure-of-earth-materials-fall-2004/lecture-notes/lec5.pdf

all uploaded online

Thank you for your attention