

Rutherford

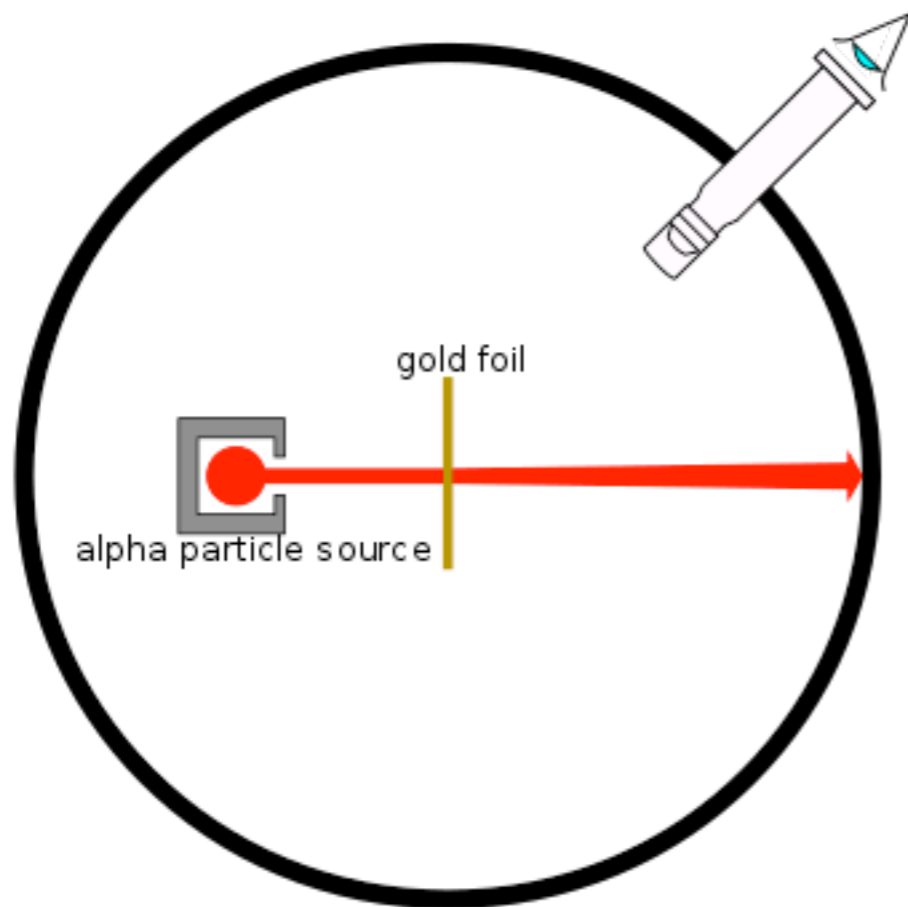
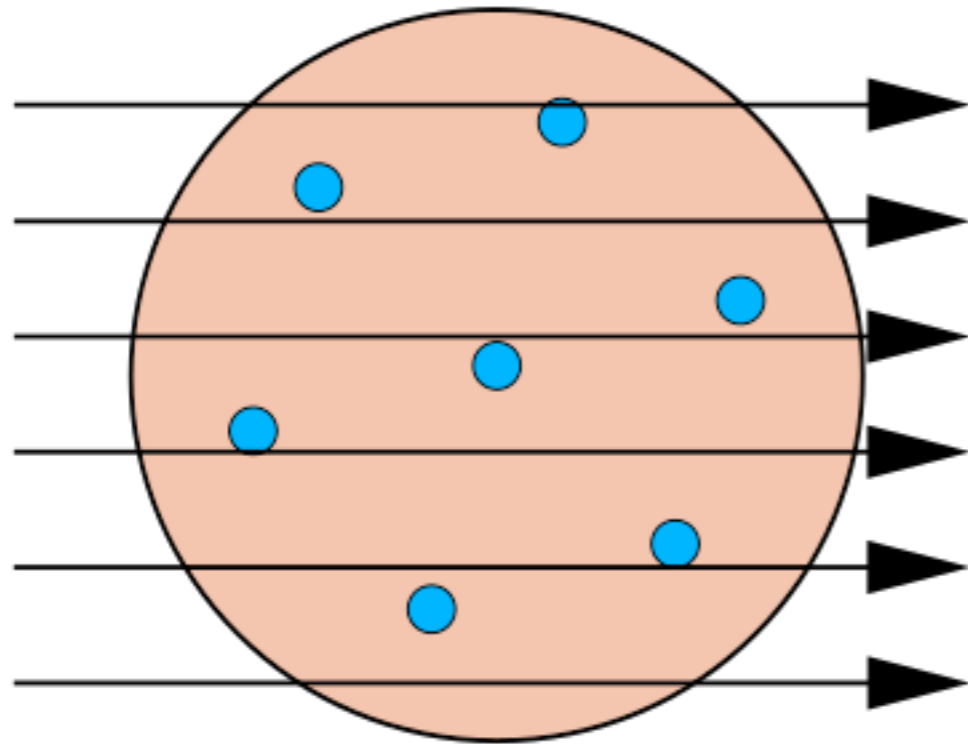


Nobelova za kemijo (1908)

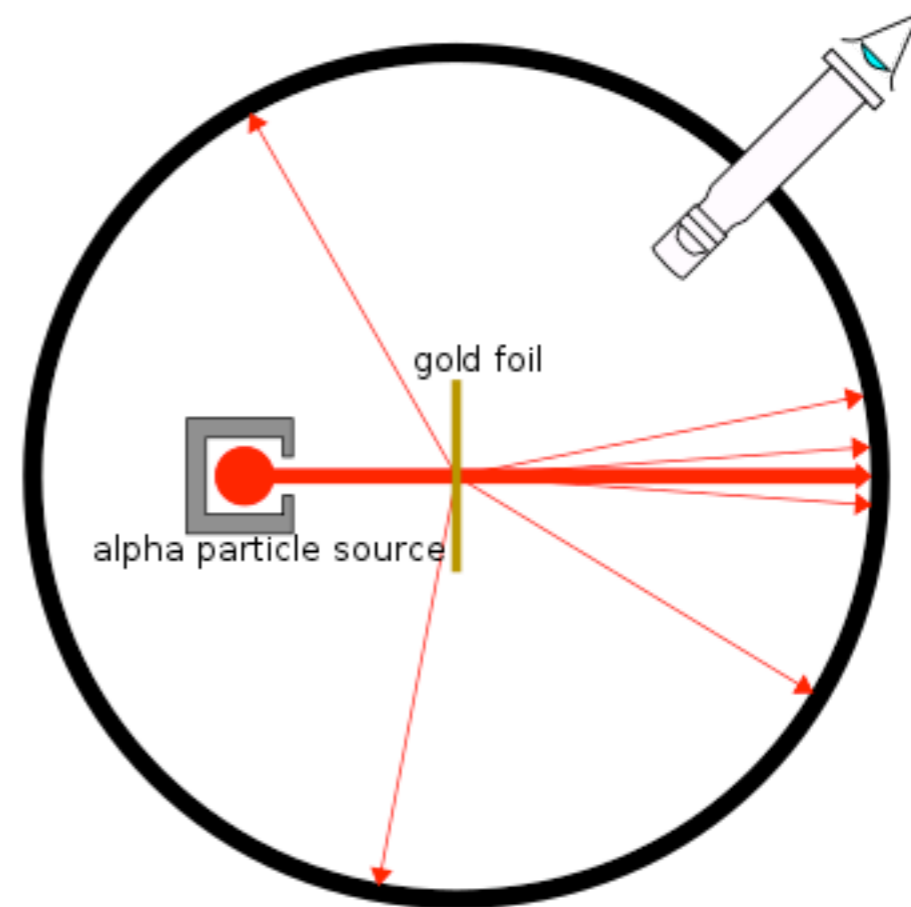
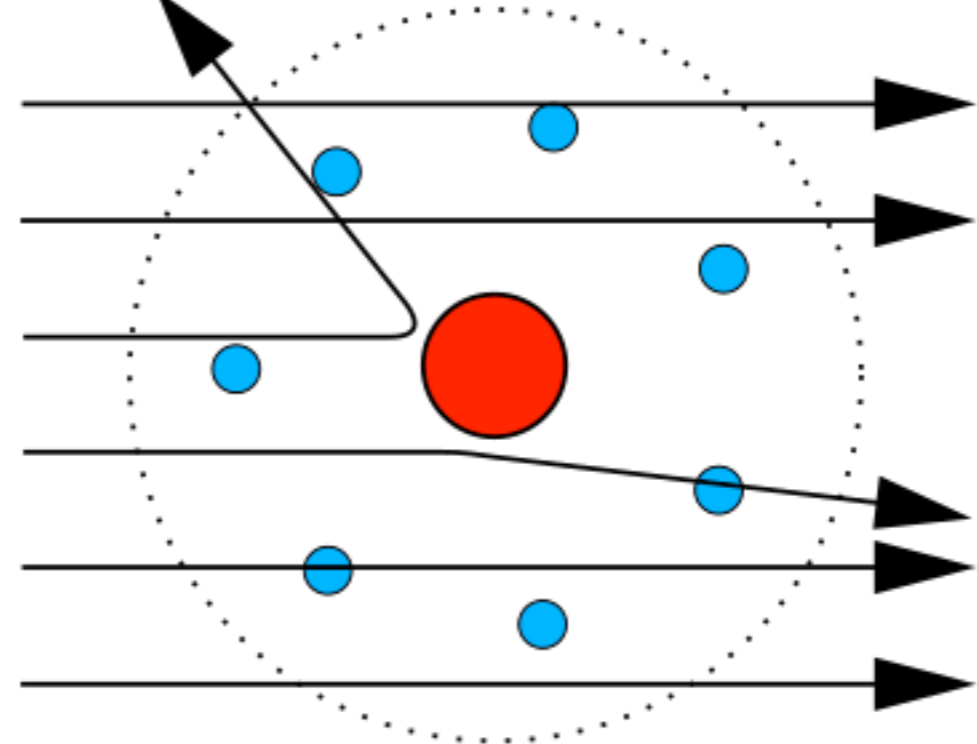
for his investigations into the
disintegration of the
elements, and the chemistry
of radioactive substances

- razpadi α , β , γ
- pojem razpolovnega časa
- razpad atoma
- **jedro atoma** (1911, Geiger in Marsden)
- jedrske reakcije ($N \rightarrow O$)
- hipoteza o protonu in nevtronu

THOMSON MODEL

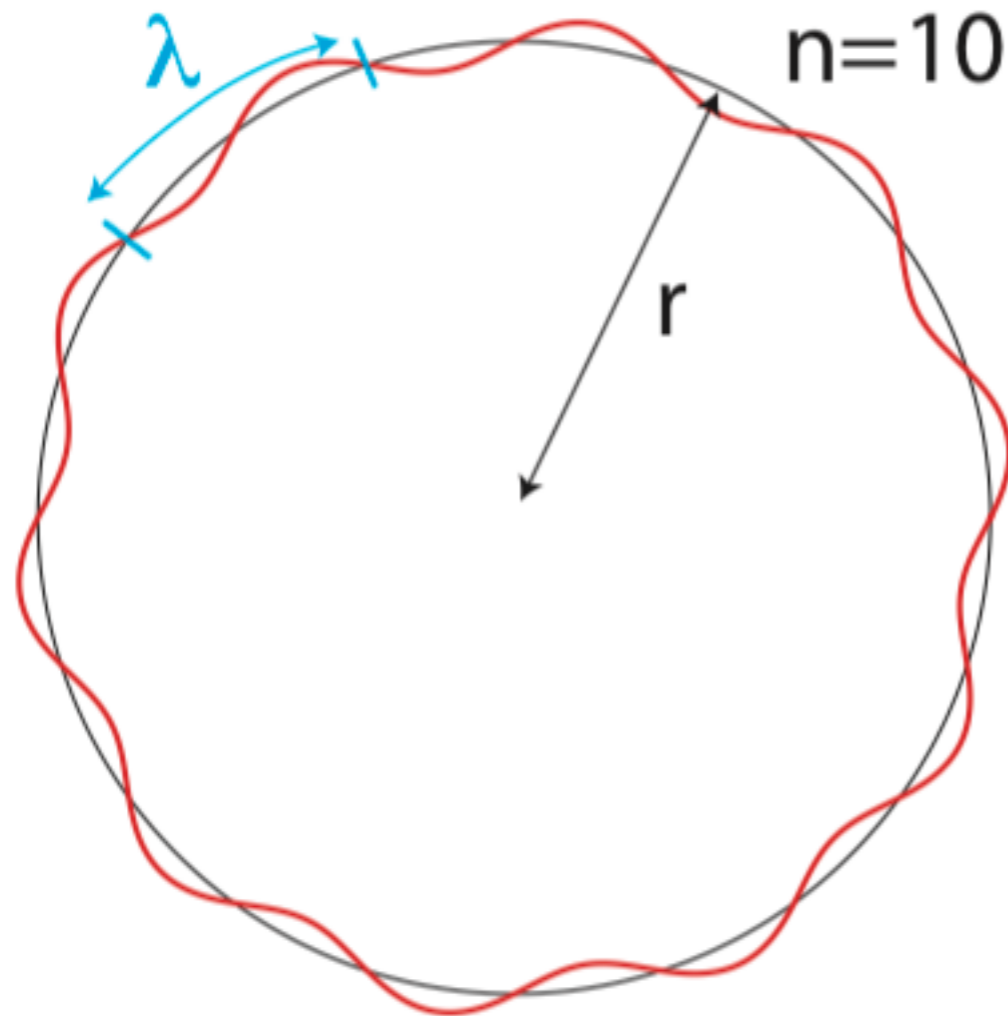


RUTHERFORD MODEL



OBSERVED RESULT

I. Predpostavke in napovedi Bohrovega modela



$$F = \frac{q_1 q_2}{4\pi\epsilon_0 r^2}$$

$$q_1 = Ze_0$$

$$q_2 = -e_0$$

$$m \frac{v^2}{r} = \frac{e_0^2}{4\pi\epsilon_0 r^2}$$

$$2\pi r = n\lambda = n \frac{h}{mv}$$

kvantizacijski pogoj

$$r_n = n^2 a_0$$

$$a_0 = \frac{4\pi\epsilon_0\hbar^2}{me_0^2} = 0,052 \text{ nm}$$

Bohrov polmer

$$E = \frac{1}{2}mv^2 - \frac{e_0^2}{4\pi\epsilon_0 r}$$

$$E_n = -\frac{1}{n^2}E_I$$

$$E_I = \frac{me_0^4}{2(4\pi\epsilon_0\hbar)^2} = 13,6 \text{ eV}$$

| Ry = | Rydberg

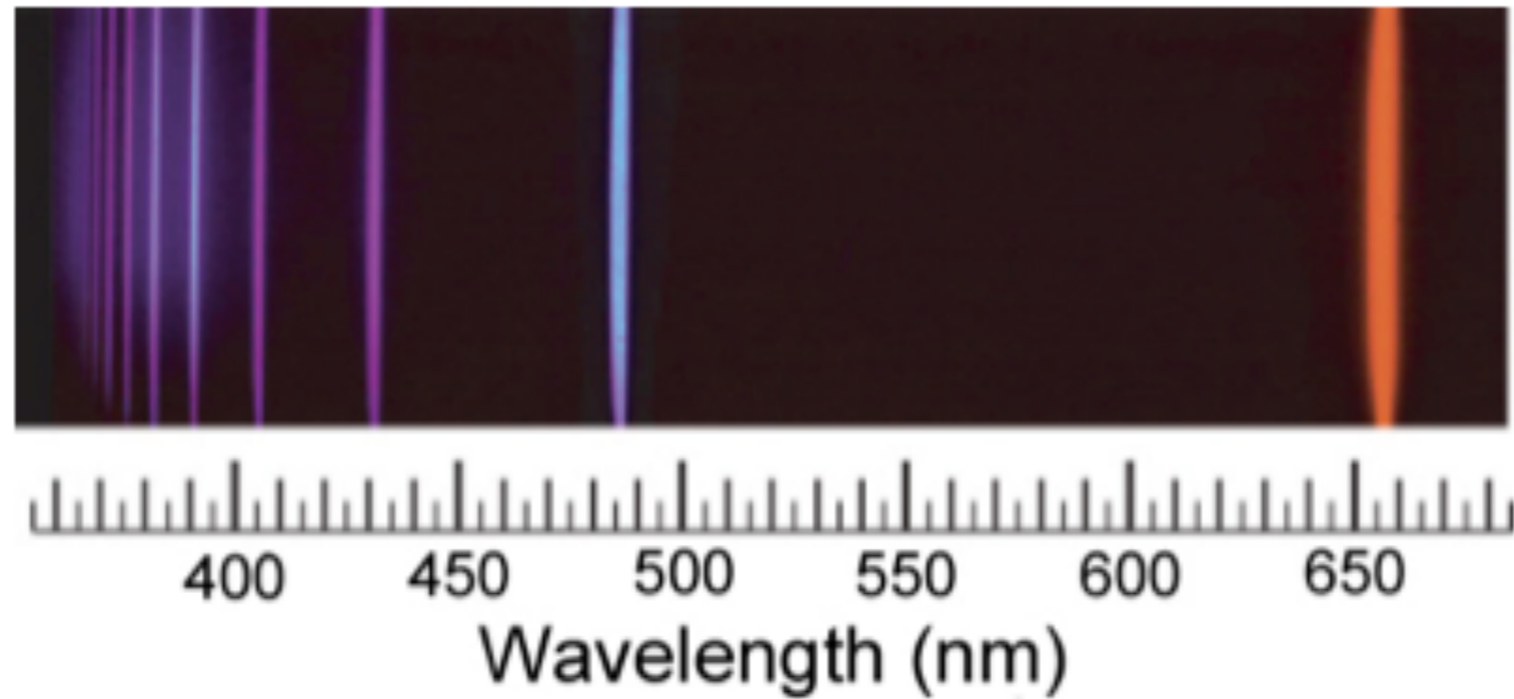
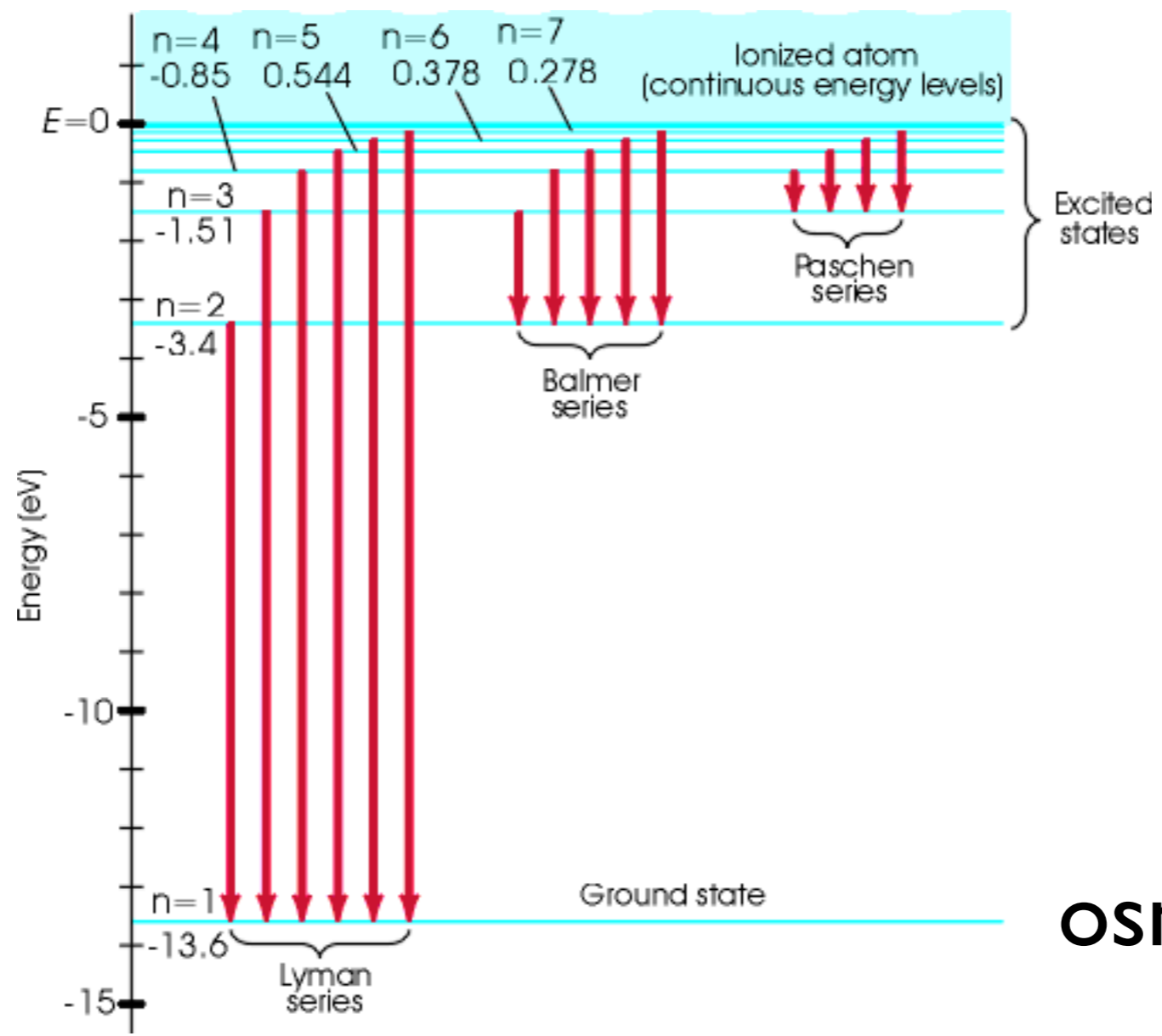
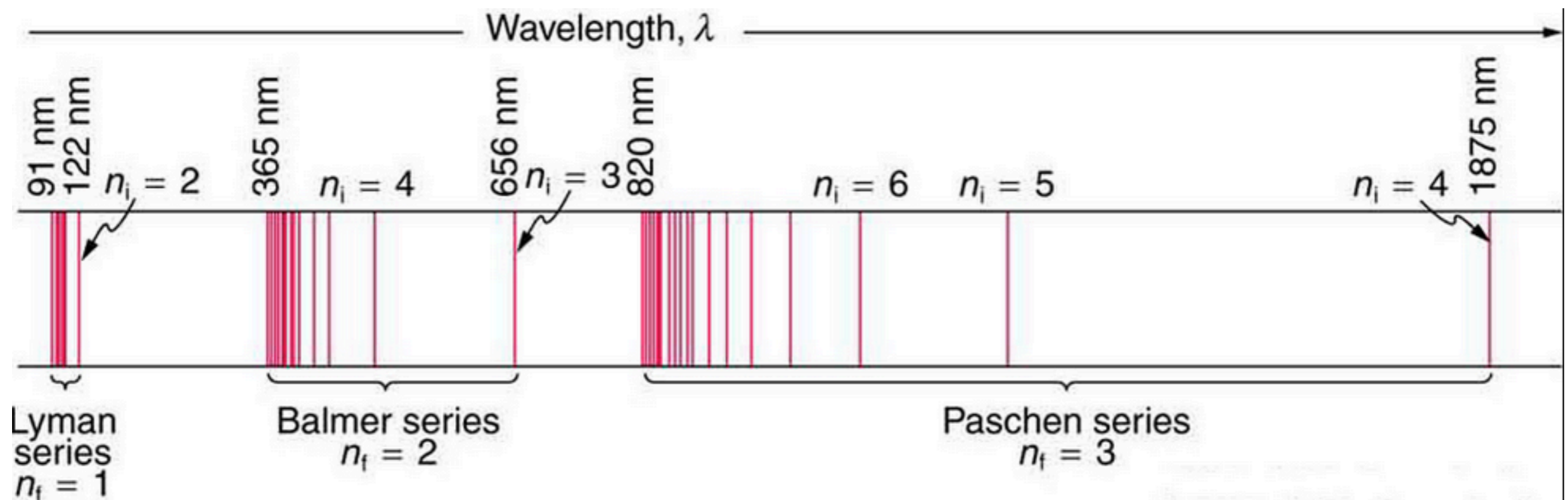


Figure 12: The spectrum of atomic hydrogen.
Source: © T.W. Hänsch.

$$h\nu = E_{n'} - E_n = E_I \left(\frac{1}{n^2} - \frac{1}{n'^2} \right)$$



osnovno stanje



2. Zakaj se lastnosti elementov ponavljajo periodično?

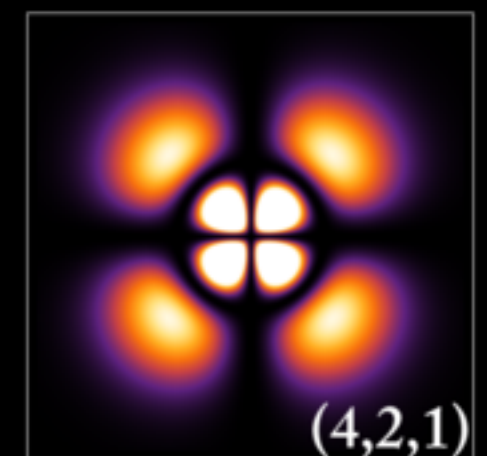
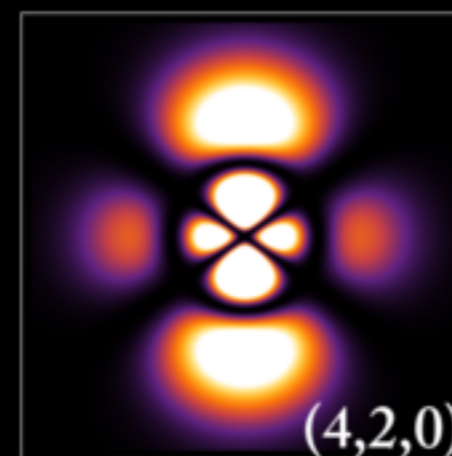
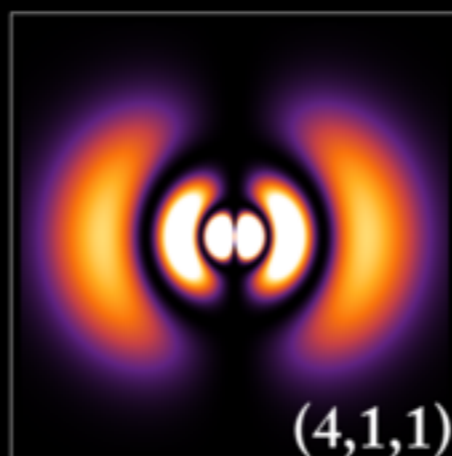
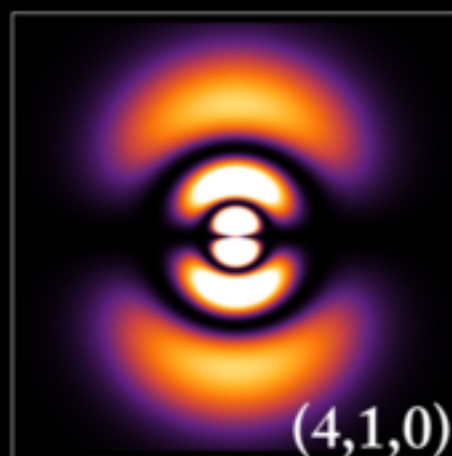
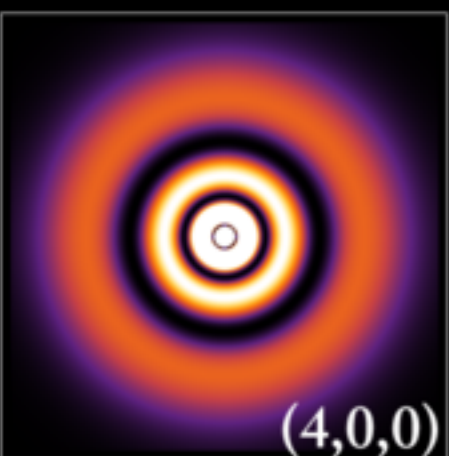
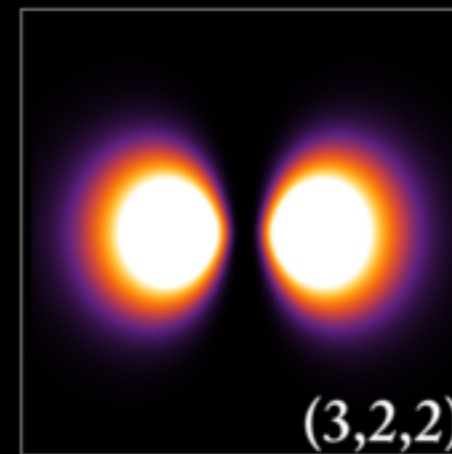
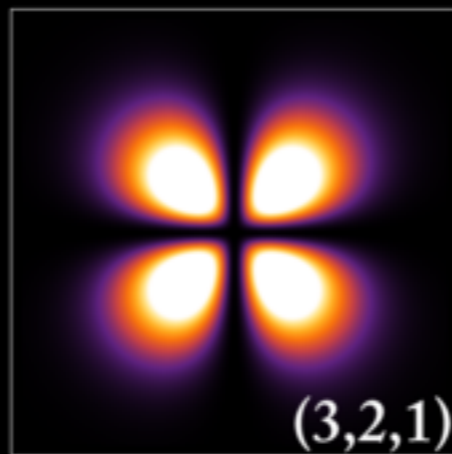
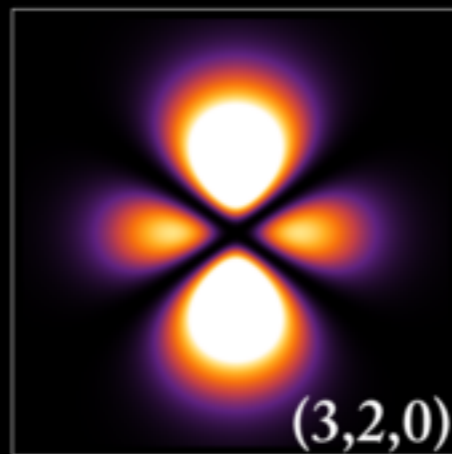
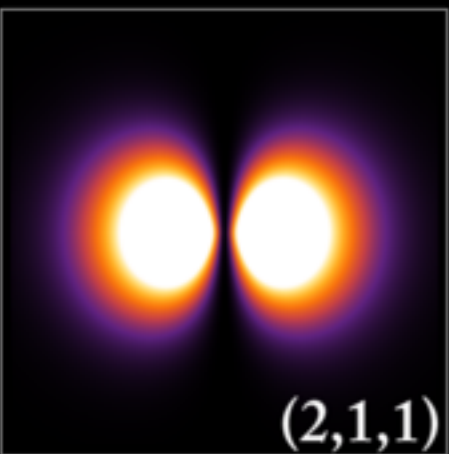
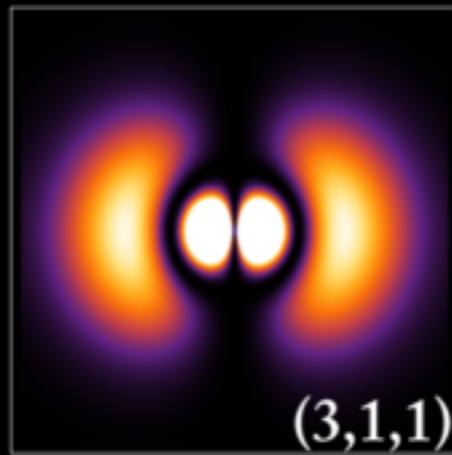
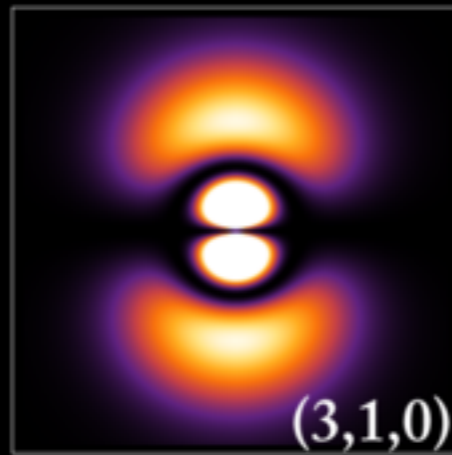
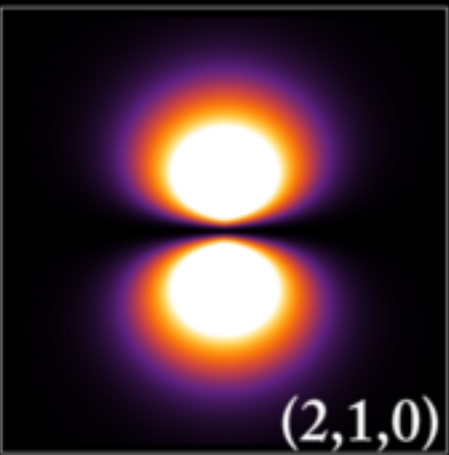
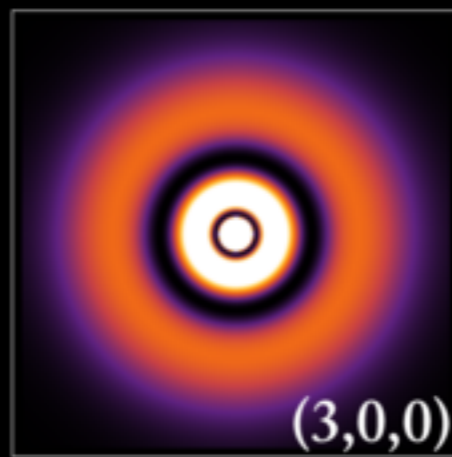
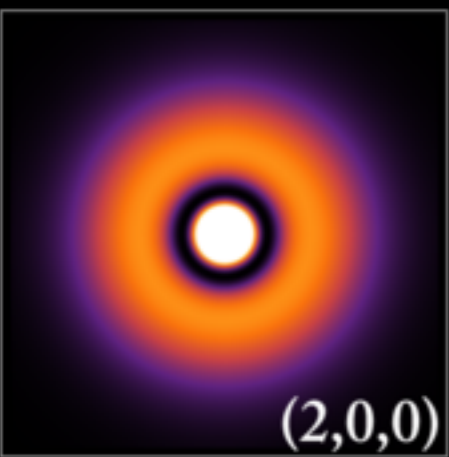
$$-\frac{\hbar^2}{2m} \left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right) - \frac{e_0^2}{4\pi\epsilon_0 r} \psi(\mathbf{r}) = E\psi(\mathbf{r})$$

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

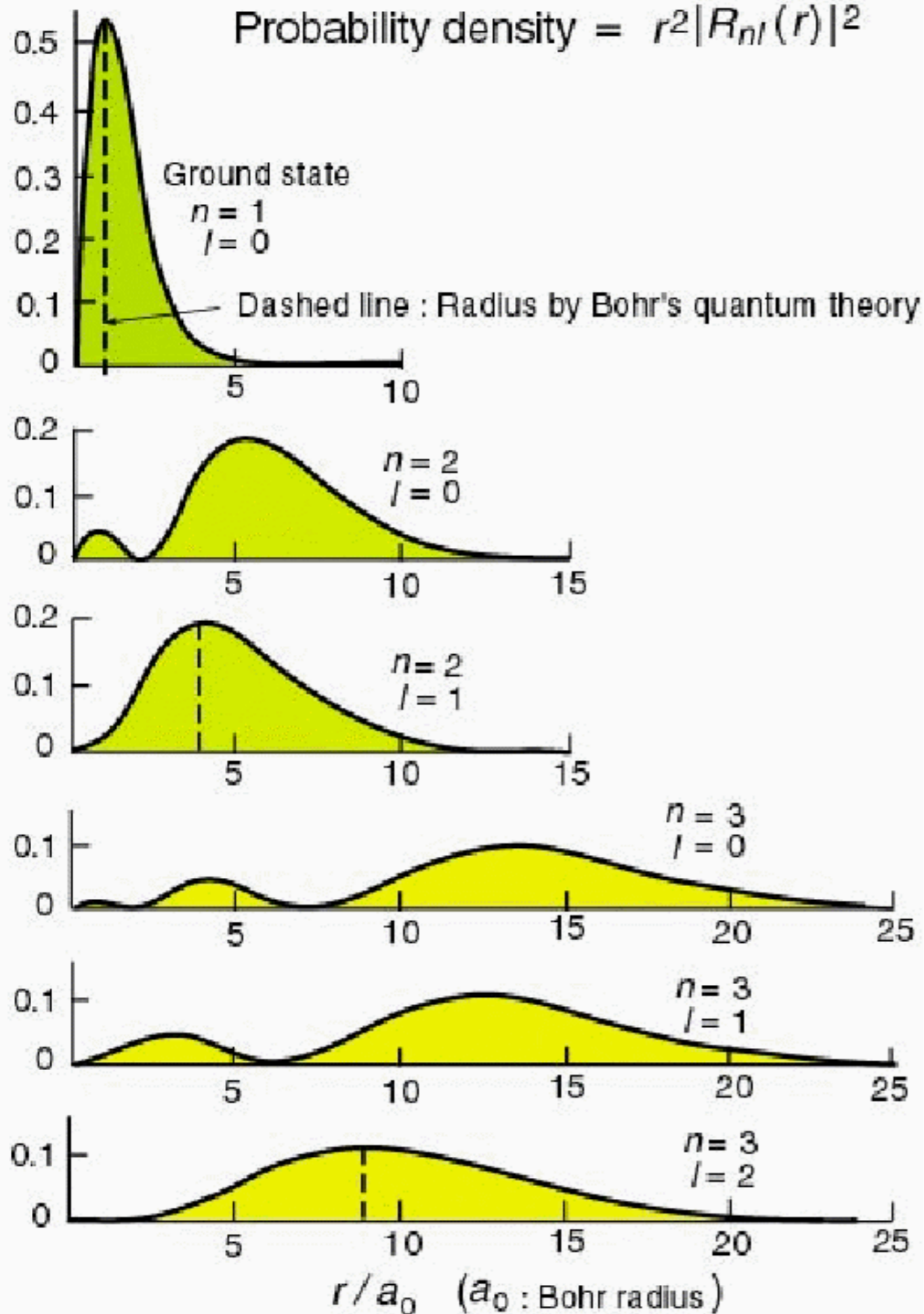
Hydrogen Wave Function

Probability density plots.

$$\psi_{nlm}(r, \vartheta, \varphi) = \sqrt{\left(\frac{2}{na_0}\right)^3 \frac{(n-l-1)!}{2n[(n+l)!]}} e^{-\rho/2} \rho^l L_{n-l-1}^{2l+1}(\rho) \cdot Y_{lm}(\vartheta, \varphi)$$



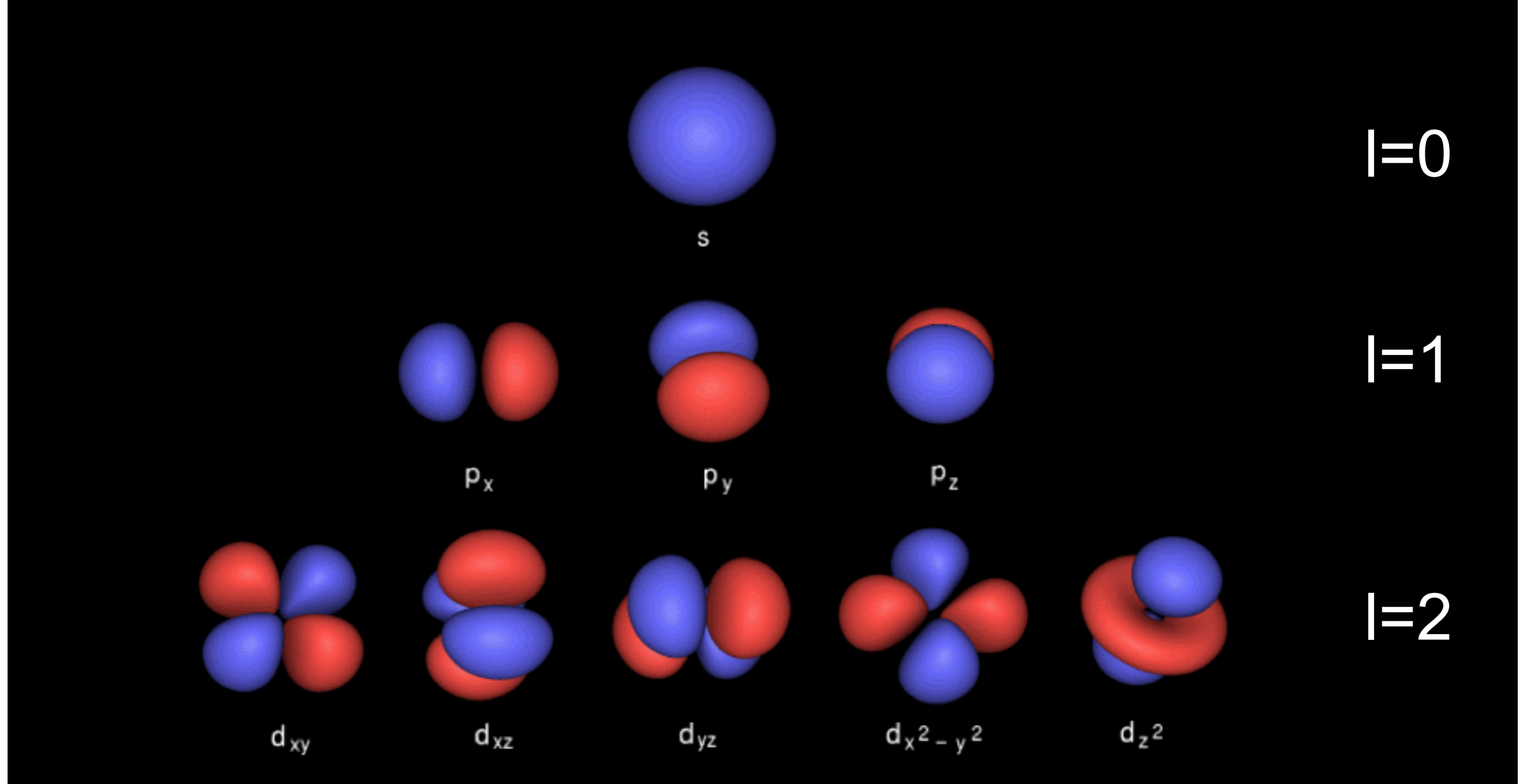
$$\text{Probability density} = r^2 |R_{nl}(r)|^2$$



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

n	oznaka
1	K
2	L
3	M
4	N

$$n_r = n - l - 1$$

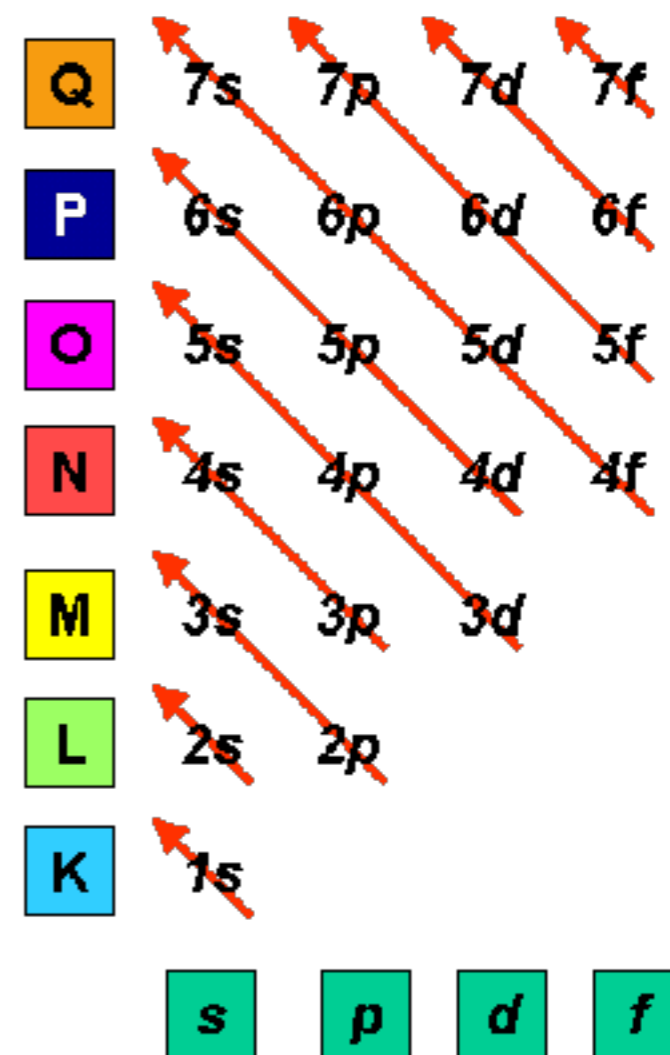


krogetelne funkcije (angl. spherical harmonics)

$$Y_{l,m}(\theta, \phi)$$

l	oznaka
0	s
1	p
2	d
3	f

perioda	podlupina	
	degeneracija	
5	5p	6
	4d	10
	5s	2
4	4p	6
	3d	10
	4s	2
3	3p	6
	3s	2
2	2p	6
	2s	2
1	1s	2



Elements by Orbital

Sequence with which the orbitals fill with electrons

Element	Configuration	1s	2s	2p _x	2p _y	2p _z	3s	3p _x	3p _y	3p _z	4s	3d	4p
H	1s ¹	↑											
He	1s ²	↑↓											
Li	1s ² 2s ¹	↑↓	↑										
Be	1s ² 2s ²	↑↓	↑↓										
B	1s ² 2s ² 2p _x ¹	↑↓	↑↓	↑									
C	1s ² 2s ² 2p _x ¹ 2p _y ¹	↑↓	↑↓	↑	↑								
N	1s ² 2s ² 2p _x ¹ 2p _y ¹ 2p _z ¹	↑↓	↑↓	↑	↑	↑							
O	1s ² 2s ² 2p _x ² 2p _y ¹ 2p _z ¹	↑↓	↑↓	↑↓	↑	↑							
F	1s ² 2s ² 2p _x ² 2p _y ² 2p _z ¹	↑↓	↑↓	↑↓	↑↓	↑							
Ne	1s ² 2s ² 2p _x ² 2p _y ² 2p _z ²	↑↓	↑↓	↑↓	↑↓	↑↓							
Na	[Ne] 3s ¹	↑↓	↑↓	↑↓	↑↓	↑↓	↑						
Mg	[Ne] 3s ²	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓						
Al	[Ne] 3s ² 3p ¹	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑					
Si	[Ne] 3s ² 3p ²	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑				
P	[Ne] 3s ² 3p ³	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑	↑			
S	[Ne] 3s ² 3p ⁴	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑			
Cl	[Ne] 3s ² 3p ⁵	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑			
Ar	[Ne] 3s ² 3p ⁶	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓			
K	[Ar] 4s ¹	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑		
Ca	[Ar] 4s ²	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓		
Sc	[Ar] 3d ¹ 4s ²	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	
Ti	[Ar] 3d ² 4s ²	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑
V	[Ar] 3d ³ 4s ²	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑
Cr	[Ar] 3d ⁵ 4s ¹	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑	↑
Mn	[Ar] 3d ⁵ 4s ²	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑
Fe	[Ar] 3d ⁶ 4s ²	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑
Co	[Ar] 3d ⁷ 4s ²	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑
Ni	[Ar] 3d ⁸ 4s ²	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑
Cu	[Ar] 3d ¹⁰ 4s ¹	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	
Zn	[Ar] 3d ¹⁰ 4s ²	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	
Ga	[Ar] 3d ¹⁰ 4s ² 4p ¹	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑

skupina 1

skupina 2

skupina 3

skupina 4

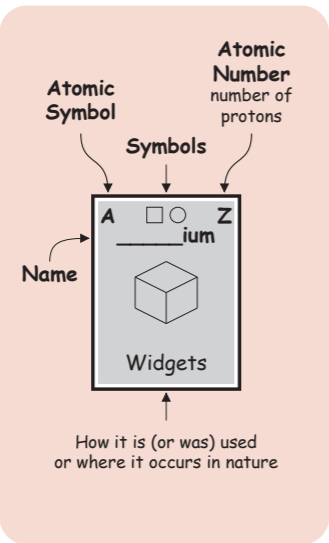
PAULIJEVO IZKLJUČITVENO NAČELO

Elektrona sta v stanjih, ki se razlikujejo vsaj v enem izmed kvantnih števil n , l , m , m_s .

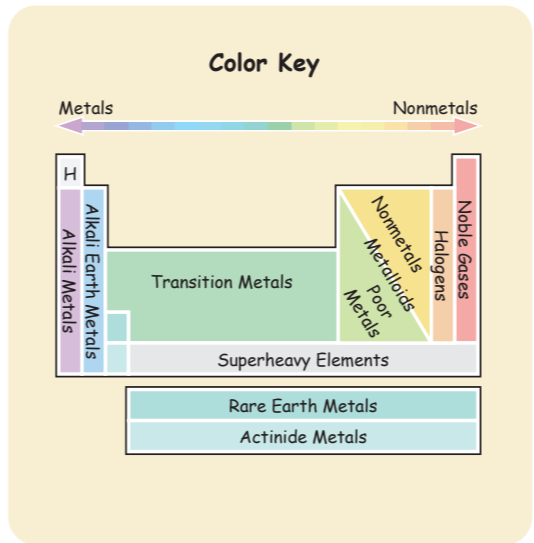
“Aufbauprinzip”




The Periodic Table of the Elements, in Pictures

Periods	Alkali Metals Group 1	Alkali Earth Metals 2	Transition Metals										Boron Group 13	Carbon Group 14	Nitrogen Group 15	Oxygen Group 16	Halogens 17	Noble Gases 18				
1	H Hydrogen Sun and Stars																	He Helium Balloons				
2	Li Lithium Batteries	Be Beryllium Emeralds											B Boron Sports Equipment	C Carbon Basis of Life's Molecules	N Nitrogen Protein	O Oxygen Air	F Fluorine Toothpaste	Ne Neon Advertising Signs				
3	Na Sodium Salt	Mg Magnesium Chlorophyll											Al Aluminum Airplanes	Si Silicon Stone, Sand, and Soil	P Phosphorus Bones	S Sulfur Egg Yolks	Cl Chlorine Swimming Pools	Ar Argon Light Bulbs				
4	K Potassium Fruits and Vegetables	Ca Calcium Shells and Bones	Sc Scandium Bicycles	Ti Titanium Aerospace	V Vanadium Springs	Cr Chromium Stainless Steel	Mn Manganese Earthmovers	Fe Iron Steel Structures	Co Cobalt Magnets	Ni Nickel Coins	Cu Copper Electric Wires	Zn Zinc Brass Instruments	Ga Gallium Light-Emitting Diodes (LEDs)	Ge Germanium Semiconductor Electronics	As Arsenic Poison	Se Selenium Copiers	Br Bromine Photography Film	Kr Krypton Flashlights				
5	Rb Rubidium Global Navigation	Sr Strontium Fireworks	Y Yttrium Lasers	Zr Zirconium Chemical Pipelines	Nb Niobium Mag Lev Trains	Mo Molybdenum Cutting Tools	Tc Technetium Radioactive Diagnosis	Ru Ruthenium Electric Switches	Rh Rhodium Searchlight Reflectors	Pd Palladium Pollution Control	Ag Silver Jewelry	Cd Cadmium Paint	In Indium Liquid Crystal Displays (LCDs)	Sn Tin Plated Food Cans	Sb Antimony Car Batteries	Te Tellurium Thermoelectric Coolers	I Iodine Disinfectant	Xe Xenon High-Intensity Lamps				
6	Cs Cesium Atomic Clocks	Ba Barium X-Ray Diagnosis	57 - 71 Rare Earth Metals		Hf Hafnium Nuclear Submarines	Ta Tantalum Mobile Phones	W Tungsten Lamp Filaments	Re Rhenium Rocket Engines	Os Osmium Pen Points	Ir Iridium Spark Plugs	Pt Platinum Labware	Au Gold Jewelry	Hg Mercury Thermometers	Tl Thallium Low-Temperature Thermometers	Pb Lead Weights	Bi Bismuth Fire Sprinklers	Po Polonium Anti-Static Brushes	At Astatine Radioactive Medicine	Rn Radon Surgical Implants			
7	Fr Francium Laser Atom Traps	Ra Radium Luminous Watches	89 - 103 Actinide Metals		Rf Rutherfordium	Db Dubnium	Sg Seaborgium	Bh Bohrium	Hs Hassium	Mt Meitnerium	Ds Darmstadtium	Rg Roentgenium	Cn Copernicium	Uut Ununtrium	Fl Flerovium	Uup Ununpentium	Lv Livermorium	Uus Ununseptium	Uuo Ununoctium			
8	119 120 121 - 153		119 120 121 - 153										119 120 121 - 153									
	Rare Earth Metals		La Lanthanum Telescope Lenses	Ce Cerium Lighter Flints	Pr Praseodymium Torchworkers' Eyeglasses	Nd Neodymium Electric Motor Magnets	Pm Promethium	Sm Samarium Electric Motor Magnets	Eu Europium Color Televisions	Gd Gadolinium MRI Diagnosis	Tb Terbium Fluorescent Lamps	Dy Dysprosium Smart Material Actuators	Ho Holmium Laser Surgery	Er Erbium Optical Fiber Communications	Tm Thulium Laser Surgery	Yb Ytterbium Scientific Fiber Lasers	Lu Lutetium Photodynamic Medicine					
	Actinide Metals		Ac Actinium Radioactive Medicine	Th Thorium Gas Lamp Mantles	Pa Protactinium Radioactive Waste	U Uranium Nuclear Power	Np Neptunium Radioactive Waste	Pu Plutonium Nuclear Weapons	Am Americium Smoke Detectors	Cm Curium Mineral Analyzers	Bk Berkelium Radioactive Waste	Cf Californium Mineral Analyzers	Es Einsteinium	Fm Fermium	Md Mendelevium	No Nobelium	Lr Lawrencium	radioactive, never found in nature, no uses except atomic research				



- Solid** (blue square)
 - Liquid** (red drop)
 - Gas** (cloud)
 - Human Body** (stick figure)
 - Earth's Crust** (globe)
 - Magnetic** (magnet)
 - Noble Metals** (crown)
 - Radioactive** (radiation symbol)
 - Only Traces Found in Nature** (magnifying glass)
 - Never Found in Nature** (X)
- The color of the symbol is the color of the element in its most common pure form.
Examples: metallic solid (blue square), red liquid (red drop), colorless gas (cloud)



H 1 Hydrogen	 <p>Atomic Weight 18.9984032 Density 1.696 g/l Melting Point -219.6 °C Boiling Point -188.12 °C</p> <p>Fluorine is a pale yellow gas that reacts violently with virtually everything, including glass. There's probably some in this fused quartz bulb (if it hasn't eaten its way out yet).</p>																He 2 Helium	
Li 3 Lithium	Be 4 Beryllium	B 5 Boron	C 6 Carbon	N 7 Nitrogen	O 8 Oxygen	F 9 Fluorine	Ne 10 Neon	Na 11 Sodium	Mg 12 Magnesium	Al 13 Aluminum	Si 14 Silicon	P 15 Phosphorus	S 16 Sulfur	Cl 17 Chlorine	Ar 18 Argon			
K 19 Potassium	Ca 20 Calcium	Sc 21 Scandium	Ti 22 Titanium	V 23 Vanadium	Cr 24 Chromium	Mn 25 Manganese	Fe 26 Iron	Co 27 Cobalt	Ni 28 Nickel	Cu 29 Copper	Zn 30 Zinc	Ga 31 Gallium	Ge 32 Germanium	As 33 Arsenic	Se 34 Selenium	Br 35 Bromine	Kr 36 Krypton	
Rb 37 Rubidium	Sr 38 Strontium	Y 39 Yttrium	Zr 40 Zirconium	Nb 41 Niobium	Mo 42 Molybdenum	Tc 43 Technetium	Ru 44 Ruthenium	Rh 45 Rhodium	Pd 46 Palladium	Ag 47 Silver	Cd 48 Cadmium	In 49 Indium	Sn 50 Tin	Sb 51 Antimony	Te 52 Tellurium	I 53 Iodine	Xe 54 Xenon	
Cs 55 Cesium	Ba 56 Barium			Hf 72 Hafnium	Ta 73 Tantalum	W 74 Tungsten	Re 75 Rhenium	Os 76 Osmium	Ir 77 Iridium	Pt 78 Platinum	Au 79 Gold	Hg 80 Mercury	Tl 81 Thallium	Pb 82 Lead	Bi 83 Bismuth	Po 84 Polonium	At 85 Astatine	Rn 86 Radon
Fr 87 Francium	Ra 88 Radium			Rf 104 Rutherfordium	Db 105 Dubnium	Sg 106 Seaborgium	Bh 107 Bohrium	Hs 108 Hassium	Mt 109 Meitnerium	Ds 110 Darmstadtium	Rg 111 Roentgenium	Cn 112 Copernicium	Uut 113 Ununtrium	Uuq 114 Ununquadium	Uup 115 Ununpentium	Uuh 116 Ununhexium	Uus 117 Ununseptium	Uuo 118 Ununoctium
La 57 Lanthanum	Ce 58 Cerium	Pr 59 Praseodymium	Nd 60 Neodymium	Pm 61 Promethium	Sm 62 Samarium	Eu 63 Europium	Gd 64 Gadolinium	Tb 65 Terbium	Dy 66 Dysprosium	Ho 67 Holmium	Er 68 Erbium	Tm 69 Thulium	Yb 70 Ytterbium	Lu 71 Lutetium				
Ac 89 Actinium	Th 90 Thorium	Pa 91 Protactinium	U 92 Uranium	Np 93 Neptunium	Pu 94 Plutonium	Am 95 Americium	Cm 96 Curium	Bk 97 Berkelium	Cf 98 Californium	Es 99 Einsteinium	Fm 100 Fermium	Md 101 Mendelevium	No 102 Nobelium	Lr 103 Lawrencium				

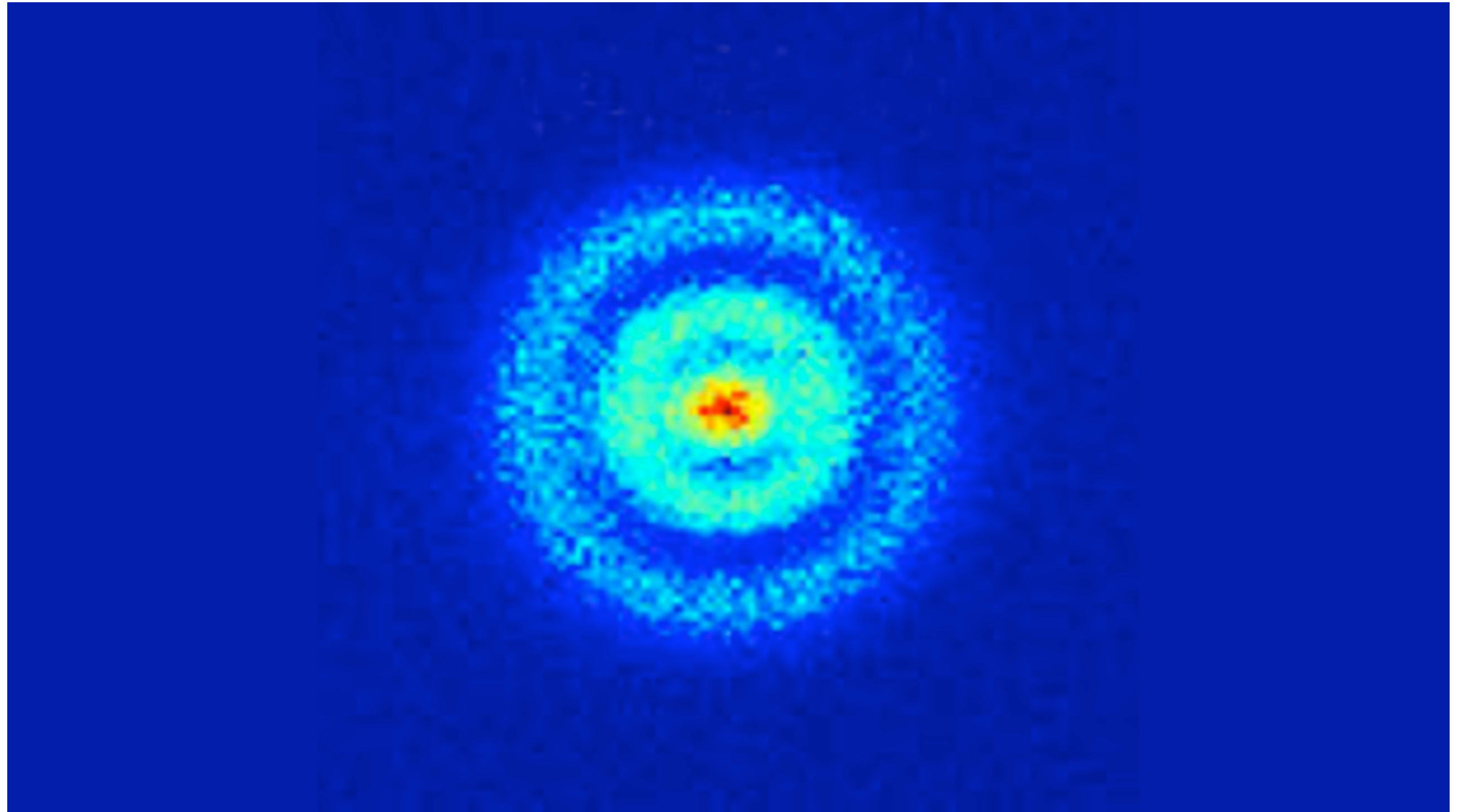
www.periodictable.com



periodic table table

(2002 Ig Nobel Prize in chemistry)





Atom vodika posnet s kvantnim mikroskopom (2013)

Kemijske vezi

The Parts of all homogeneal hard Bodies which fully touch one another, stick together very strongly. And for explaining how this may be, some have invented hooked Atoms, which is begging the Question; and others tell us that Bodies are glued together by rest, that is, by an occult Quality, or rather by nothing; and others, that they stick together by conspiring Motions, that is, by relative rest amongst themselves. I had rather infer from their Cohesion, that their Particles attract one another by some Force, which **in immediate Contact is exceeding strong, at small distances performs the chymical Operations above-mention'd, and reaches not far from the Particles with any sensible Effect.**

Newton (Opticks, 1704)

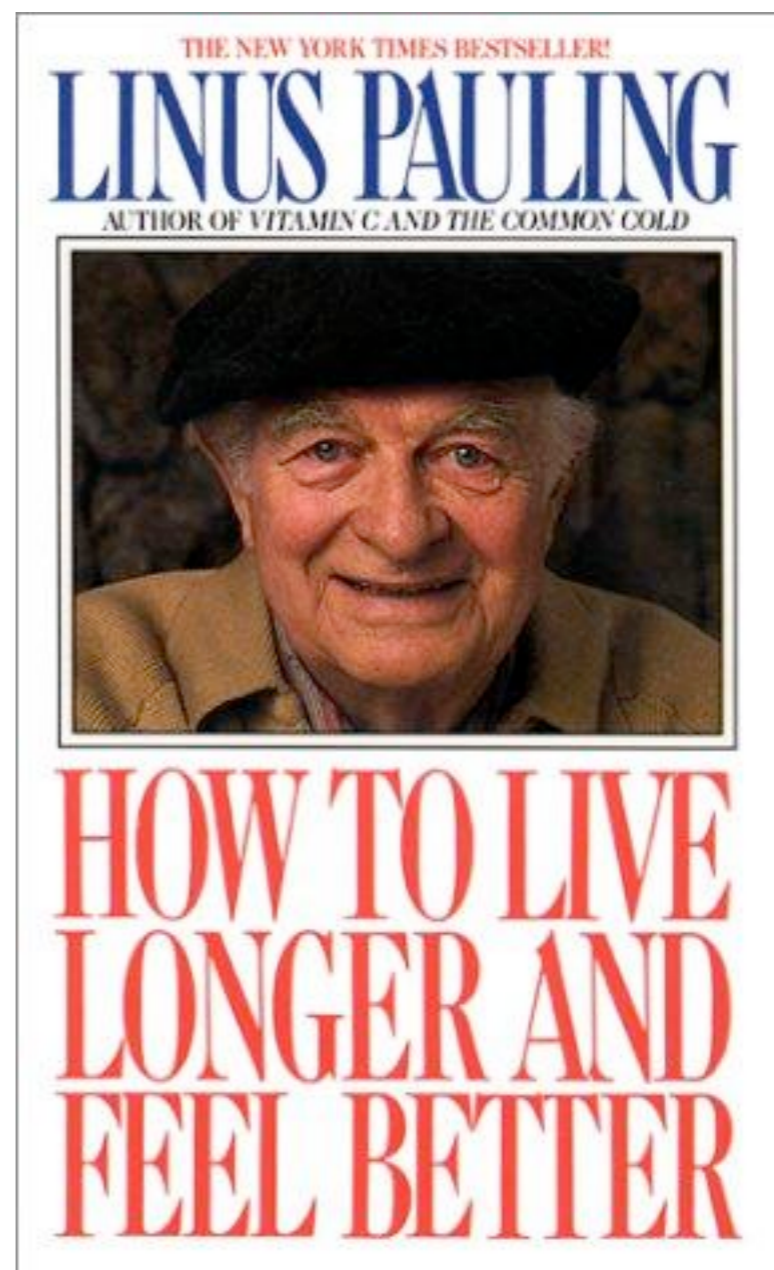
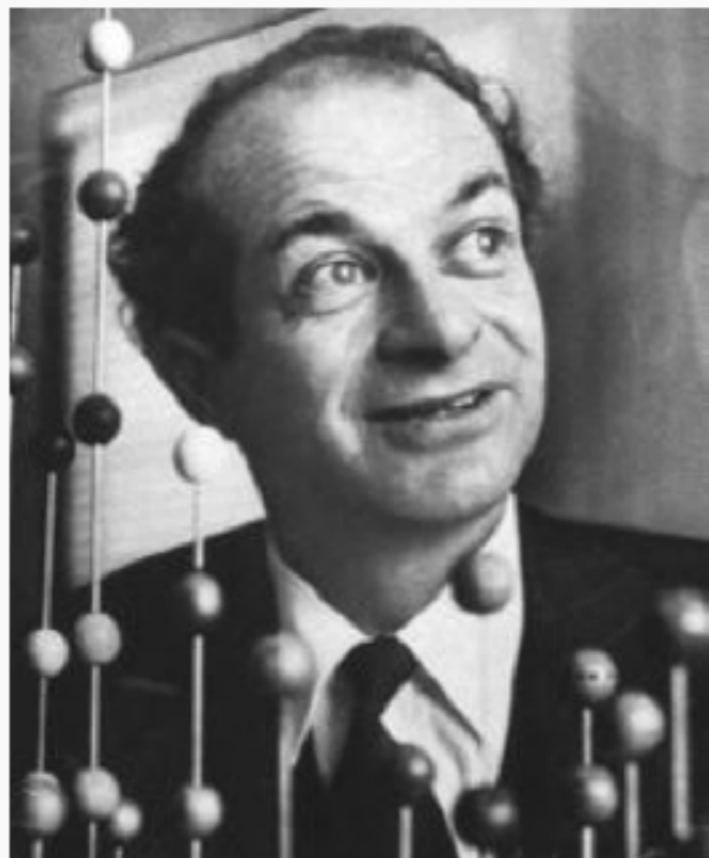


kemija

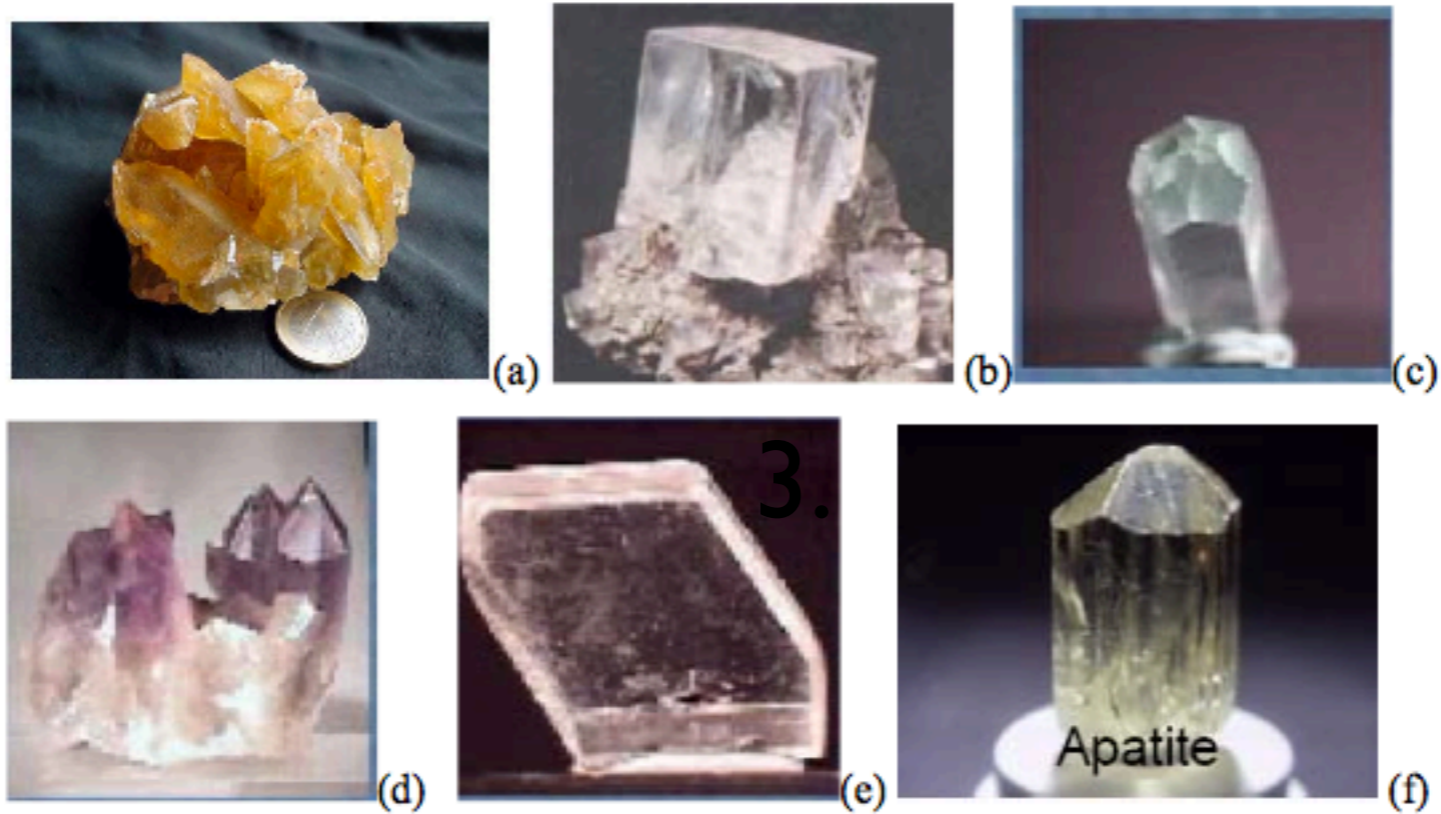


mir

Linus Pauling

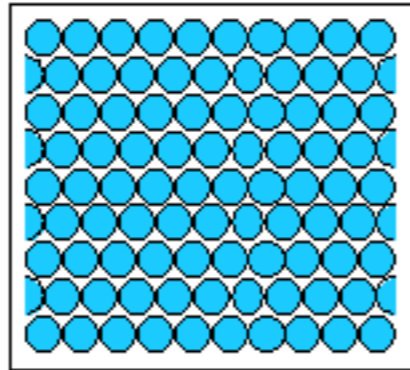


3. Kako opišemo kristalno mrežo?



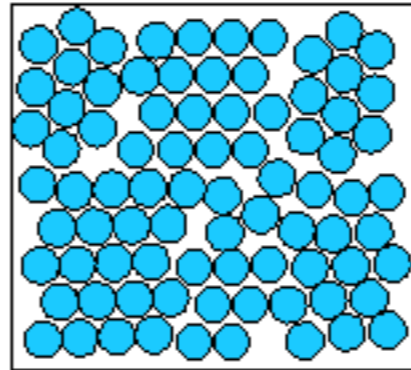
Crystals of (a) baryt, (b) salt, (c) hexagonal beryl, (d) trigonal quartz, (e) monoclinic gypsum, and apatite (f)

<http://webmineral.com/>



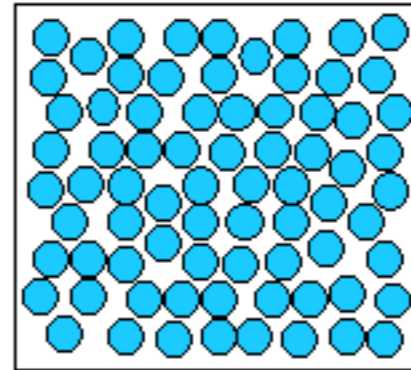
Single crystal

Periodic across the whole volume.



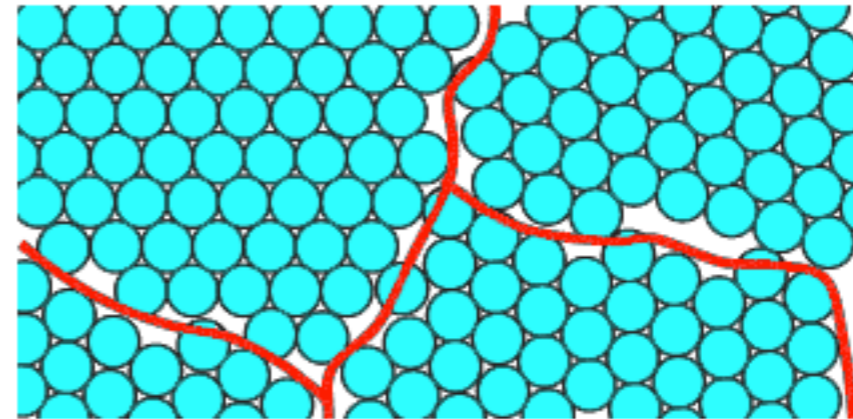
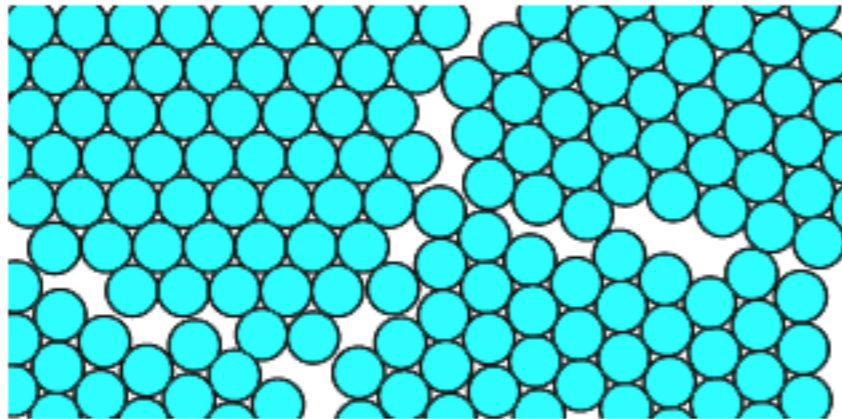
Polycrystal

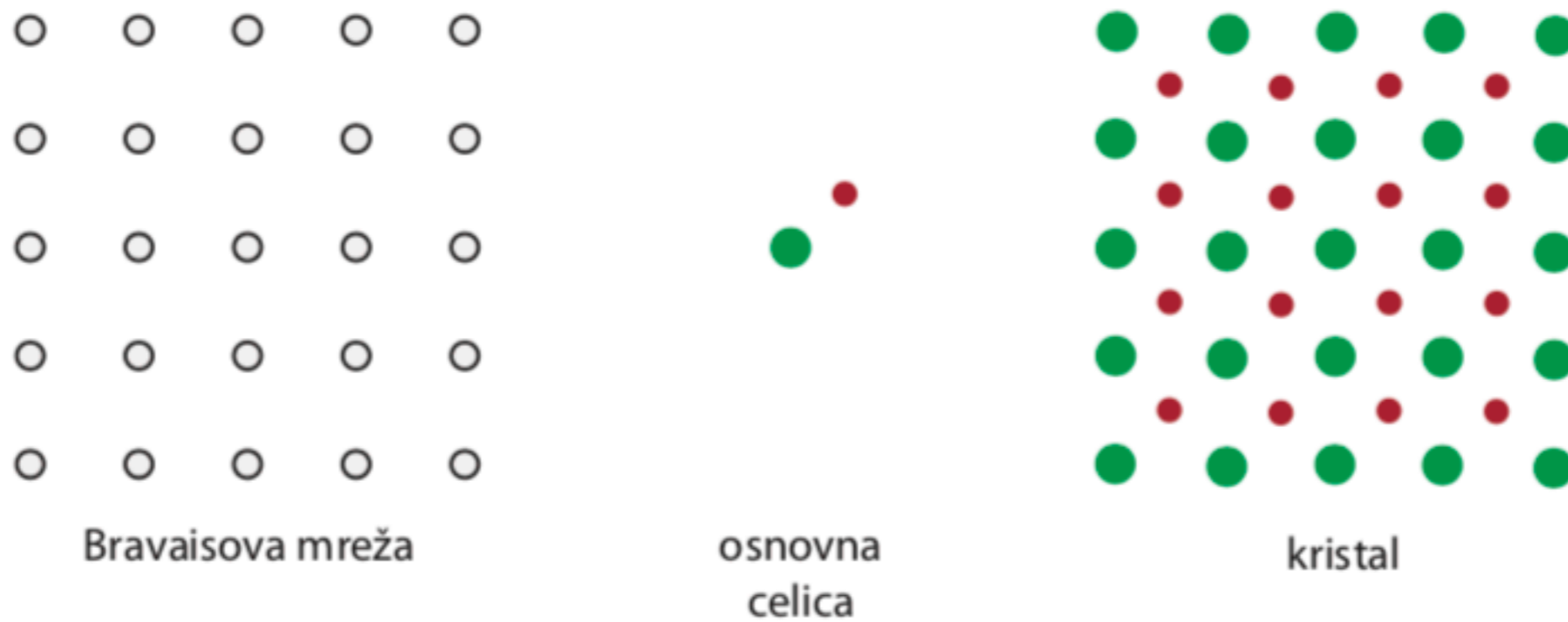
Periodic across each grain.



Amorphous solid

Not periodic.



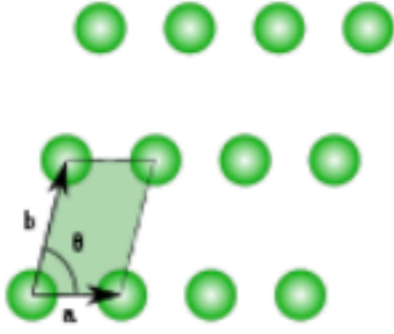
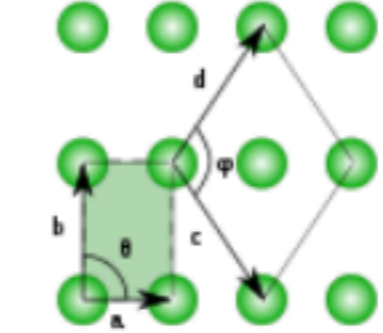
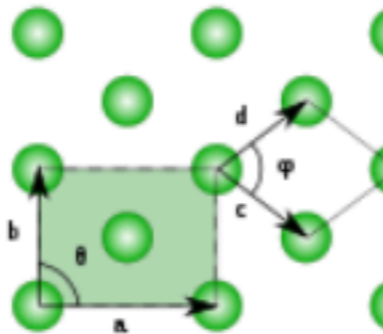
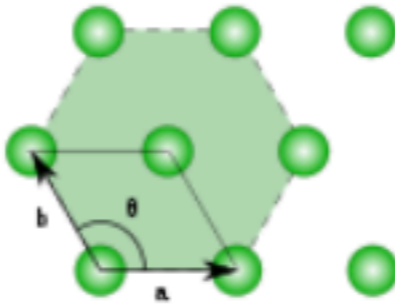
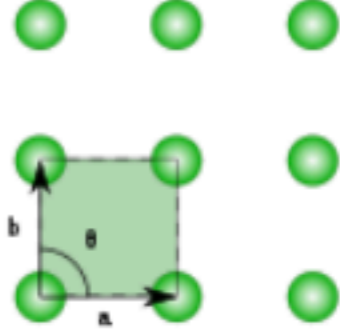



Slika 9.5. Kristalna mreža = Bravaisova mreža + baza (atomi v osnovni celici).

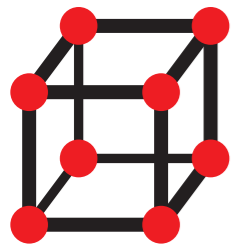
$$\mathbf{R} = u_1 \mathbf{a}_1 + u_2 \mathbf{a}_2 + u_3 \mathbf{a}_3$$

$$\mathbf{r}_j = x_j \mathbf{a}_1 + y_j \mathbf{a}_2 + z_j \mathbf{a}_3$$

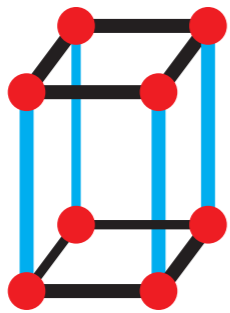
, $0 \leq x_j, y_j, z_j < 1$, saj so atomi baze znotraj *enotske celice*.

 <p>1</p>	 <p>2</p>  <p>3</p>	 <p>4</p>	 <p>5</p>
<p>$a \neq b , \theta \neq 90^\circ$</p> <p>m</p>	<p>$a \neq b , \theta = 90^\circ$ $c = d , \varphi \neq 90^\circ$</p> <p>o</p>	<p>$a = b , \theta = 120^\circ$</p> <p>h</p>	<p>$a = b , \theta = 90^\circ$</p> <p>t</p>
<p>1 – oblique (monoclinic), 2 – rectangular (orthorhombic), 3 – centered rectangular (orthorhombic), 4 – hexagonal, and 5 – square (tetragonal). </p>			

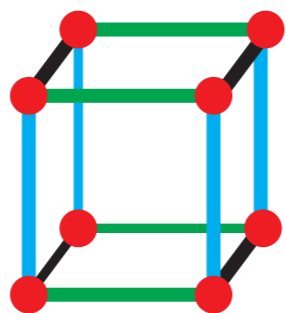
7 sistemov:



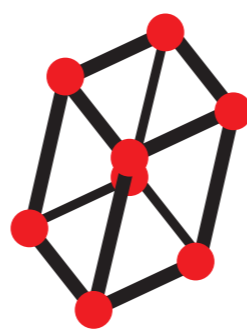
kubični
 $a=b=c$
 $\alpha=\beta=\gamma=90^\circ$



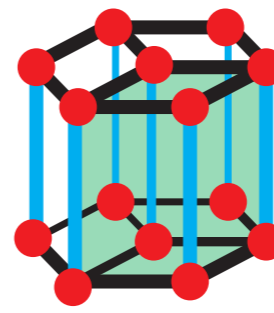
tetragonalni
 $a=b \neq c$
 $\alpha=\beta=\gamma=90^\circ$



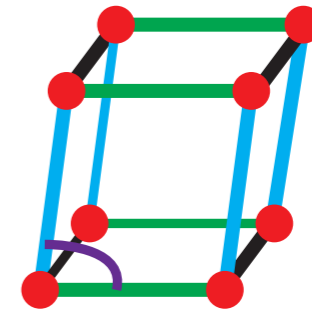
ortorombski
 $a \neq b \neq c$
 $\alpha=\beta=\gamma=90^\circ$



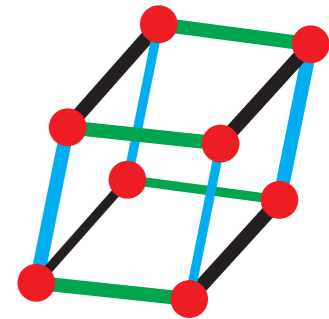
romboedrični
 $a=b=c$
 $\alpha=\beta=\gamma \neq 90^\circ$



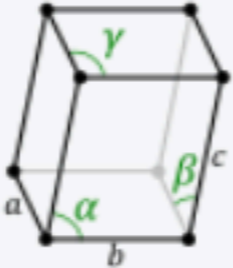
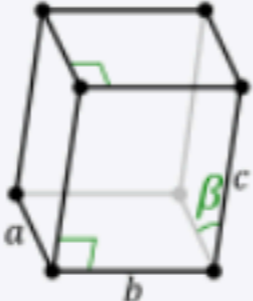
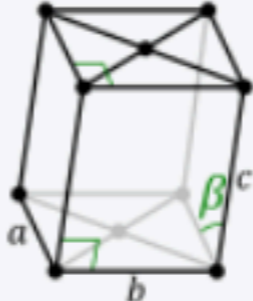
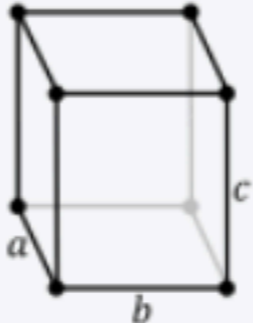
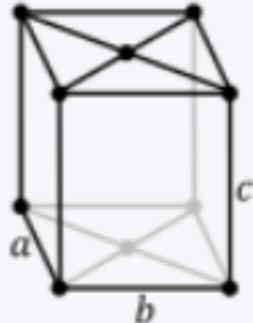
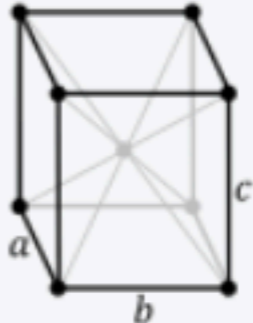
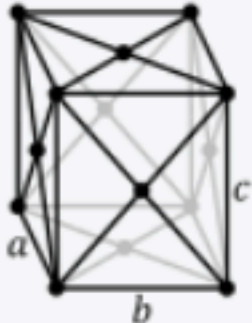
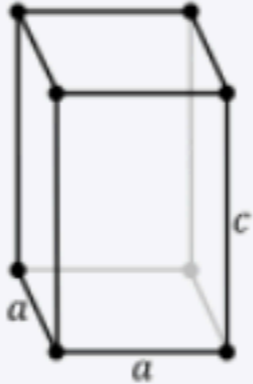
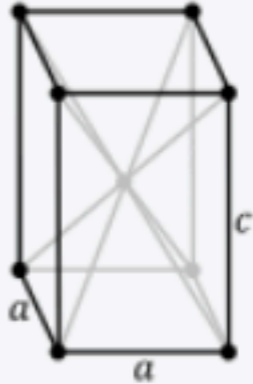
heksagonalni
 $a=b \neq c$
 $\alpha=\gamma=90^\circ$
 $\beta=120^\circ$

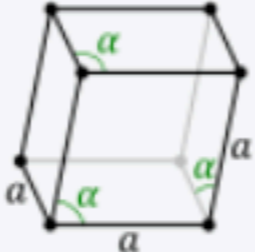
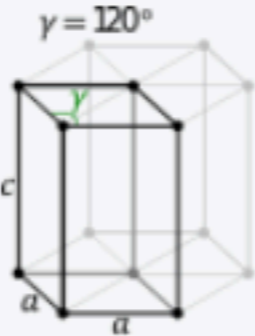
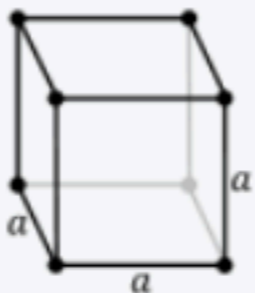
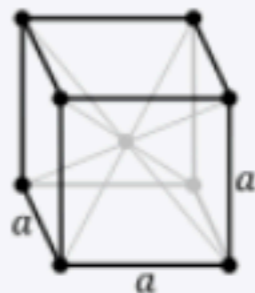
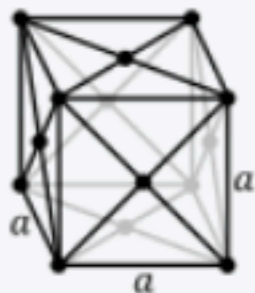


monoklinski
 $a \neq b \neq c$
 $\alpha=\gamma=90^\circ \neq \beta$

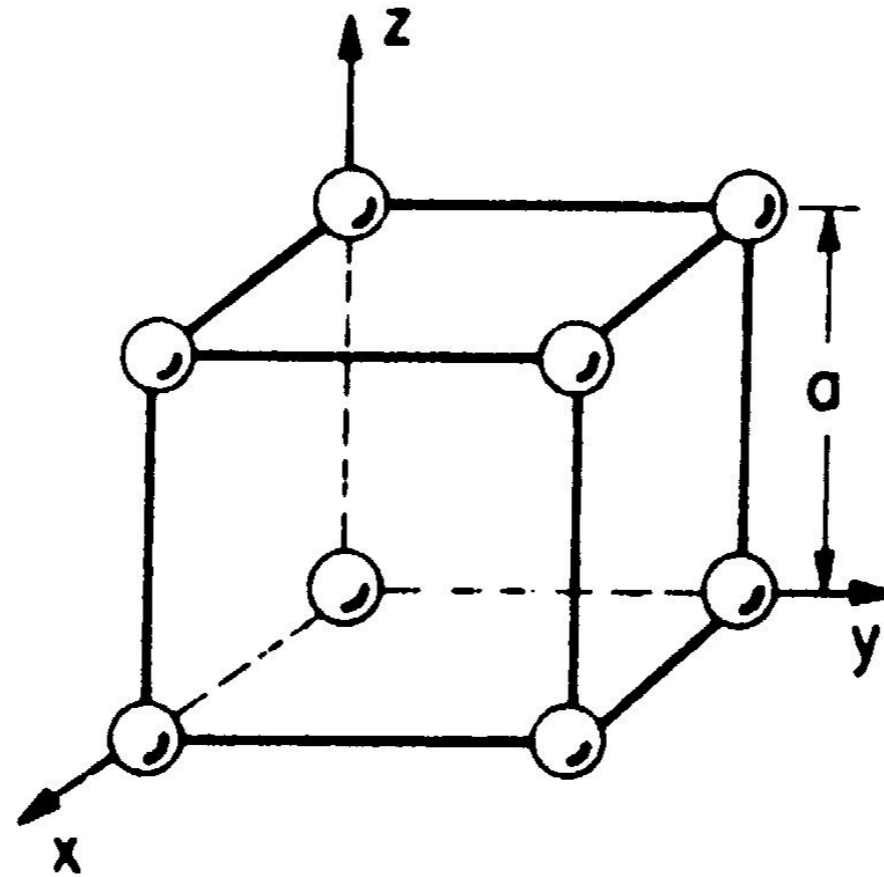


triklinski
 $a \neq b \neq c$
 $\alpha \neq \beta \neq \gamma$

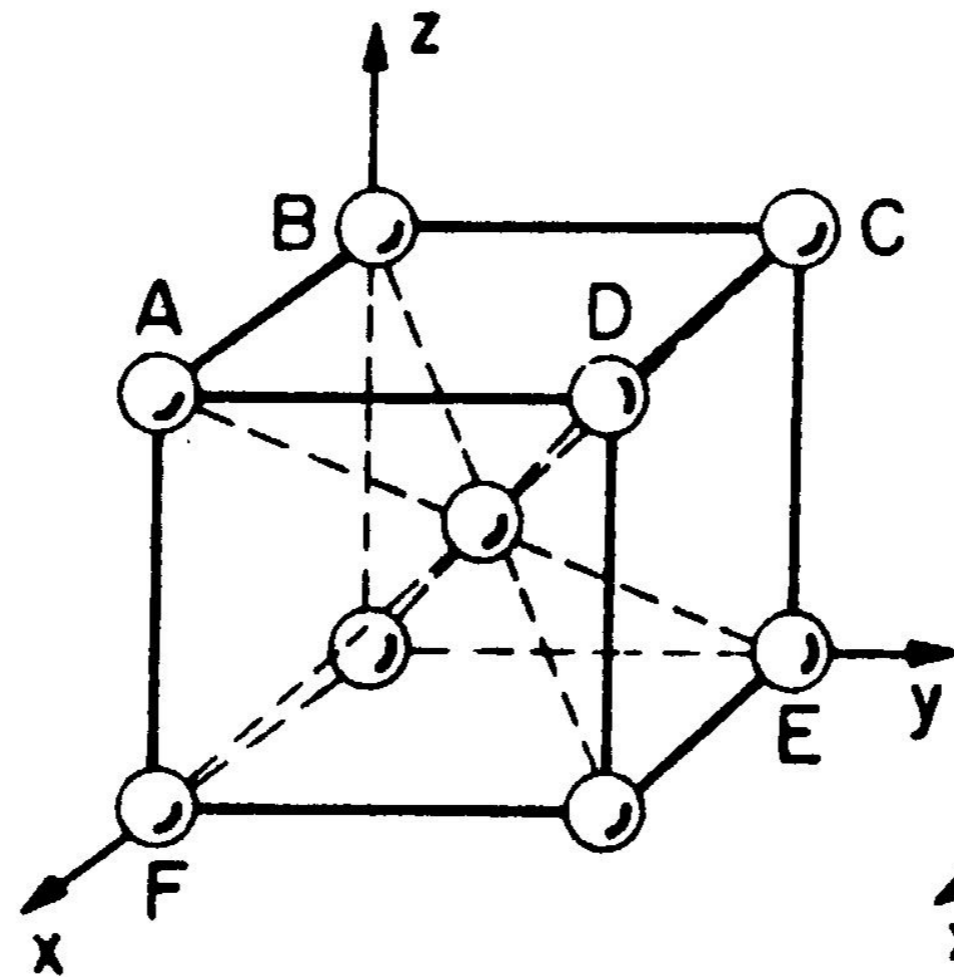
Crystal family	Lattice system	Schönflies	14 Bravais lattices			
			Primitive (P)	Base-centered (C)	Body-centered (I)	Face-centered (F)
Triclinic		C_i				
Monoclinic		C_{2h}				
Orthorhombic		D_{2h}				
Tetragonal		D_{4h}				

Hexagonal	Rhombohedral	D_{3d}				
	Hexagonal	D_{6h}	<p>$\gamma = 120^\circ$</p> 			
Cubic		O_h				

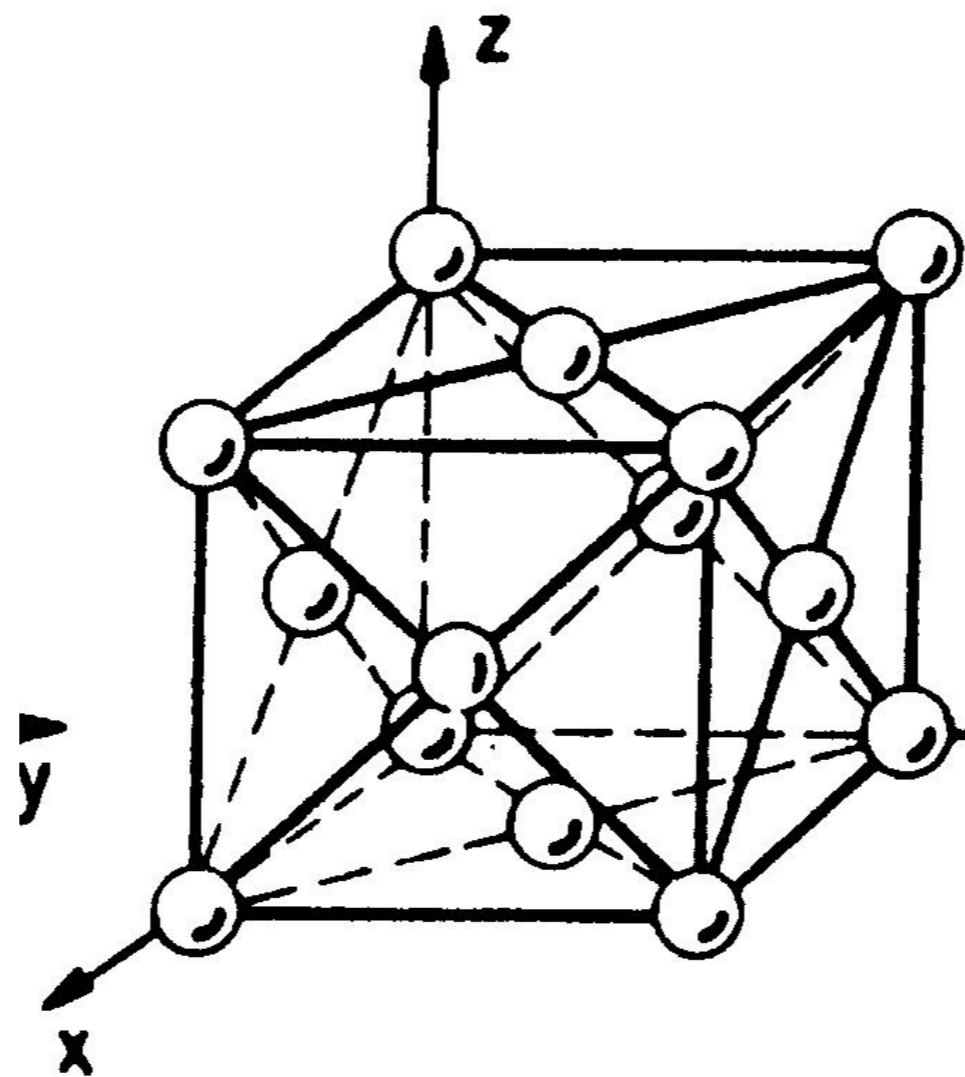
kubični



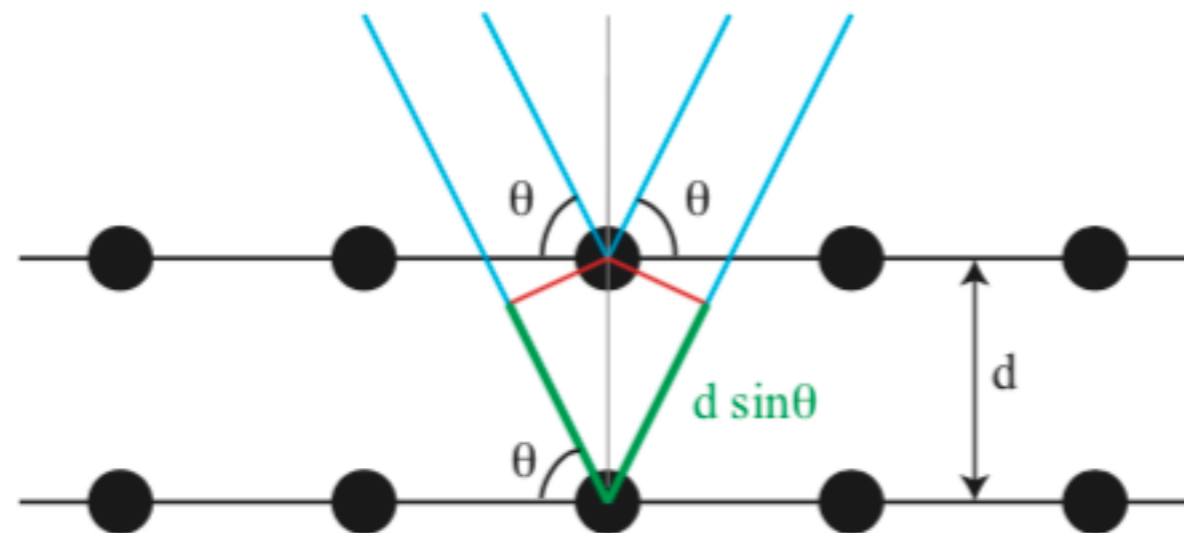
telesno centriran kubični



ploskovno centriran kubični



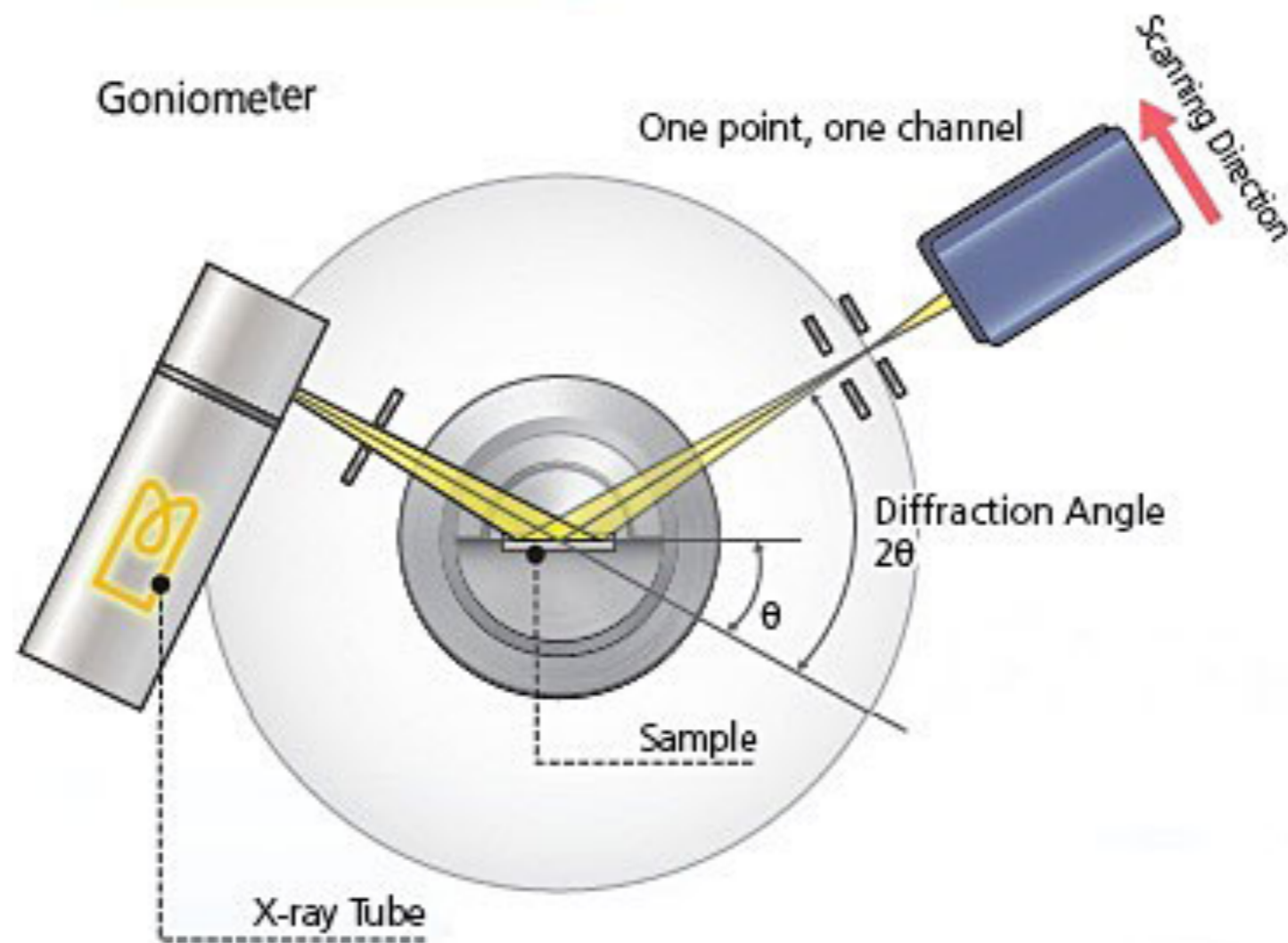
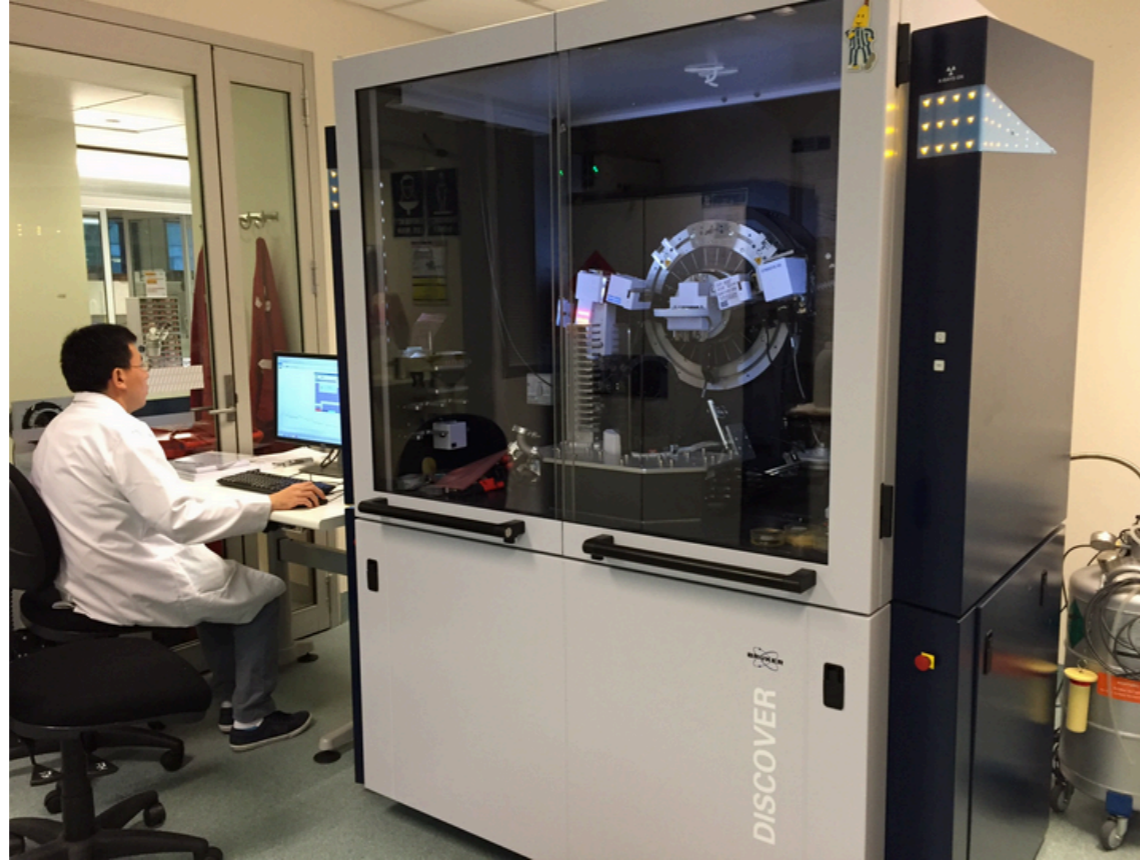
4. Kako določamo kristalno strukturo? uklon rentgenski žarkov

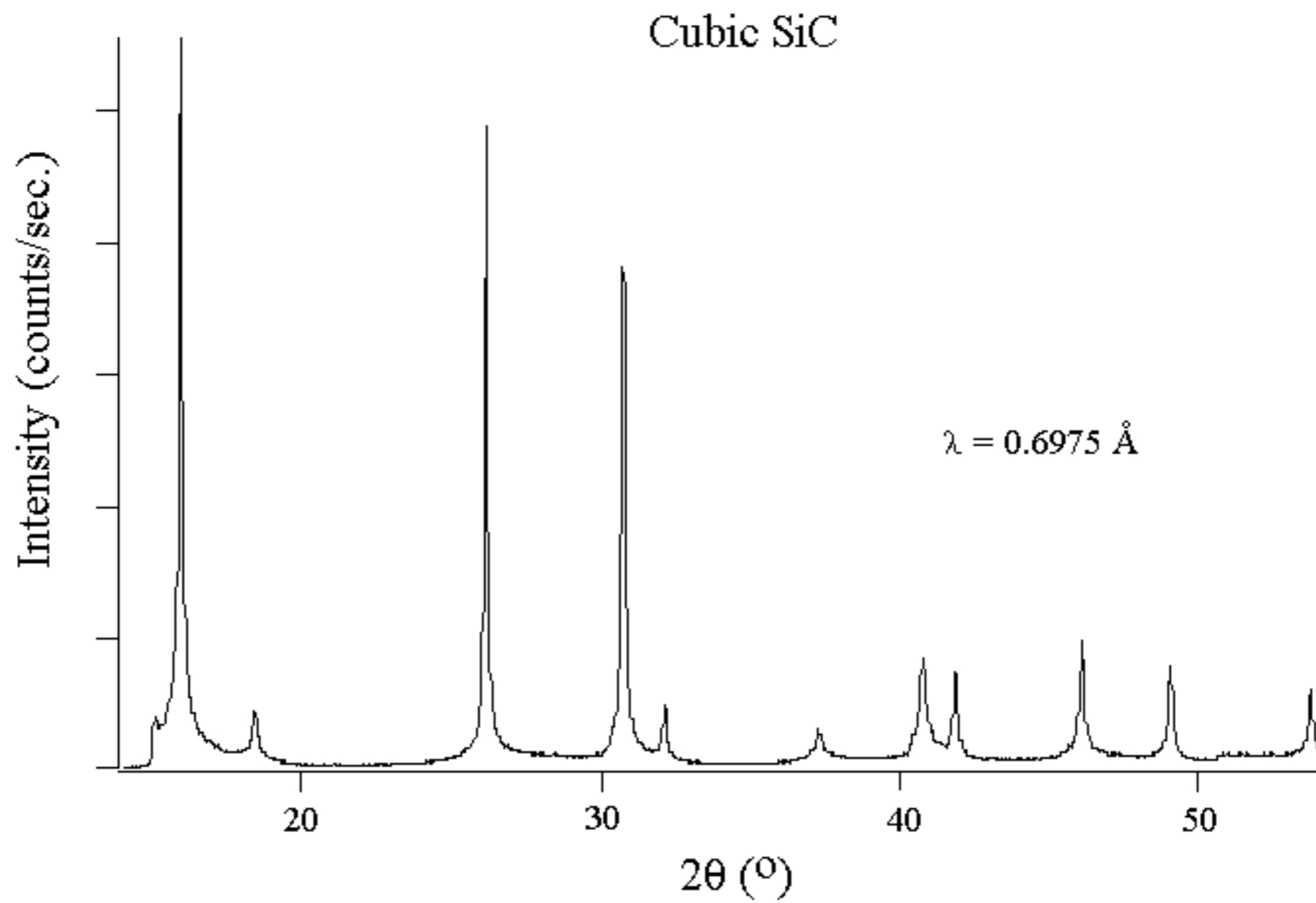


$$n\lambda = 2d \sin \theta$$

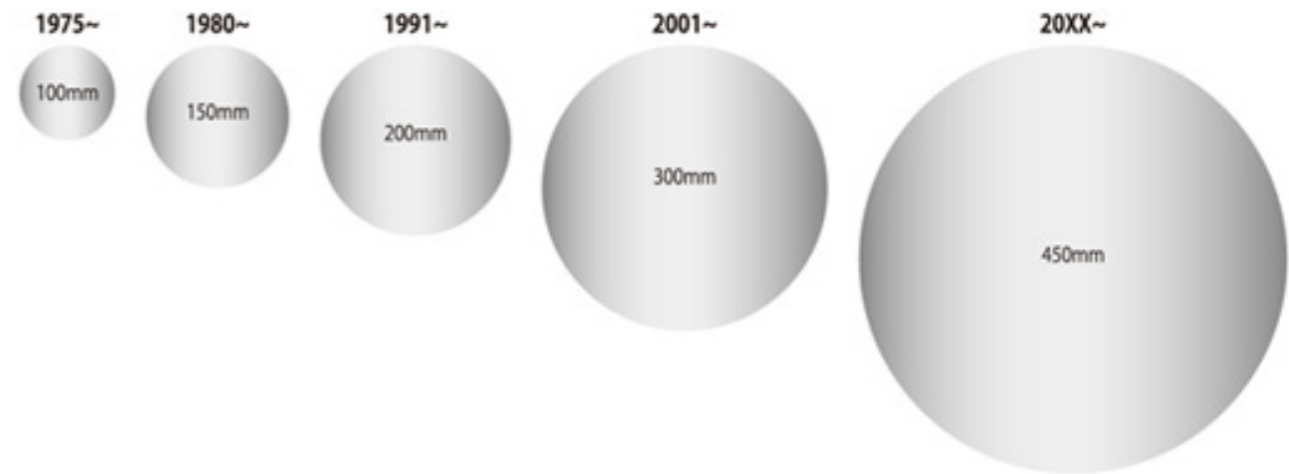
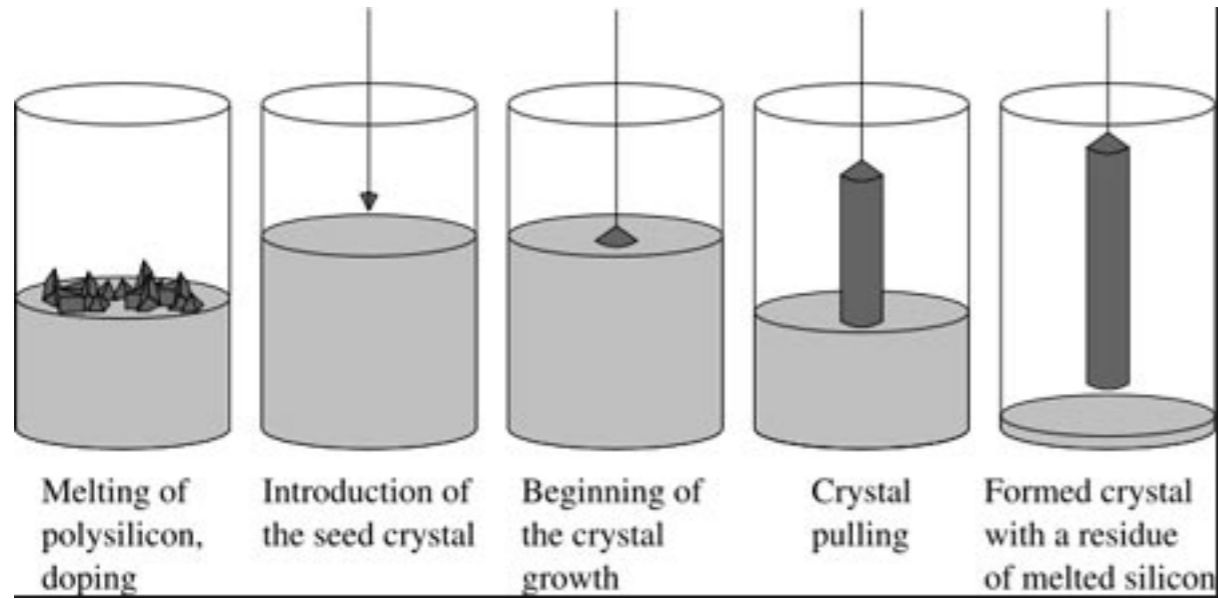
Bragg, Laue, ~1912

θ sipalni kot

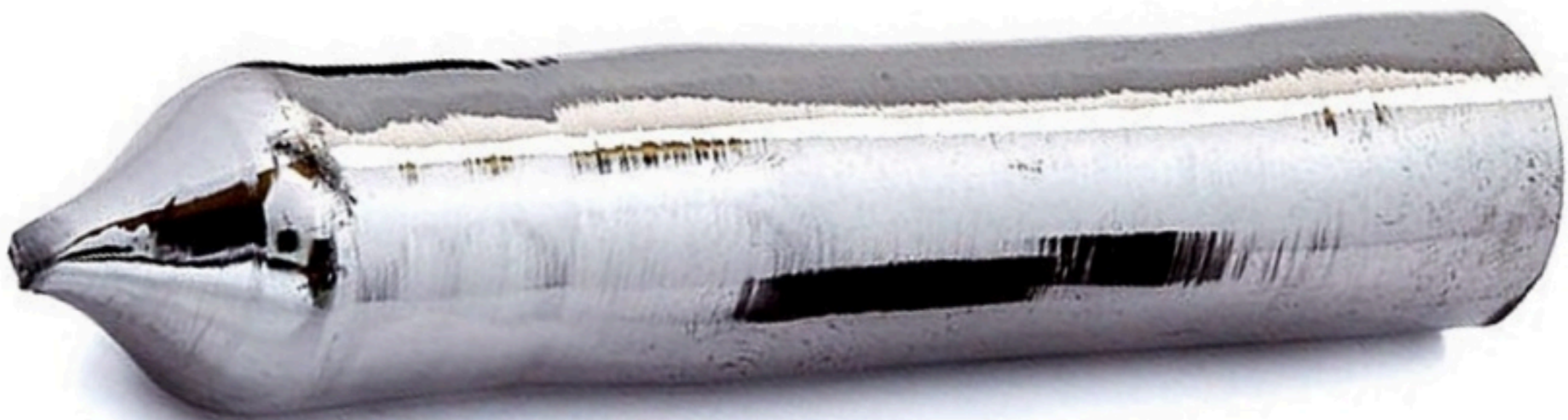


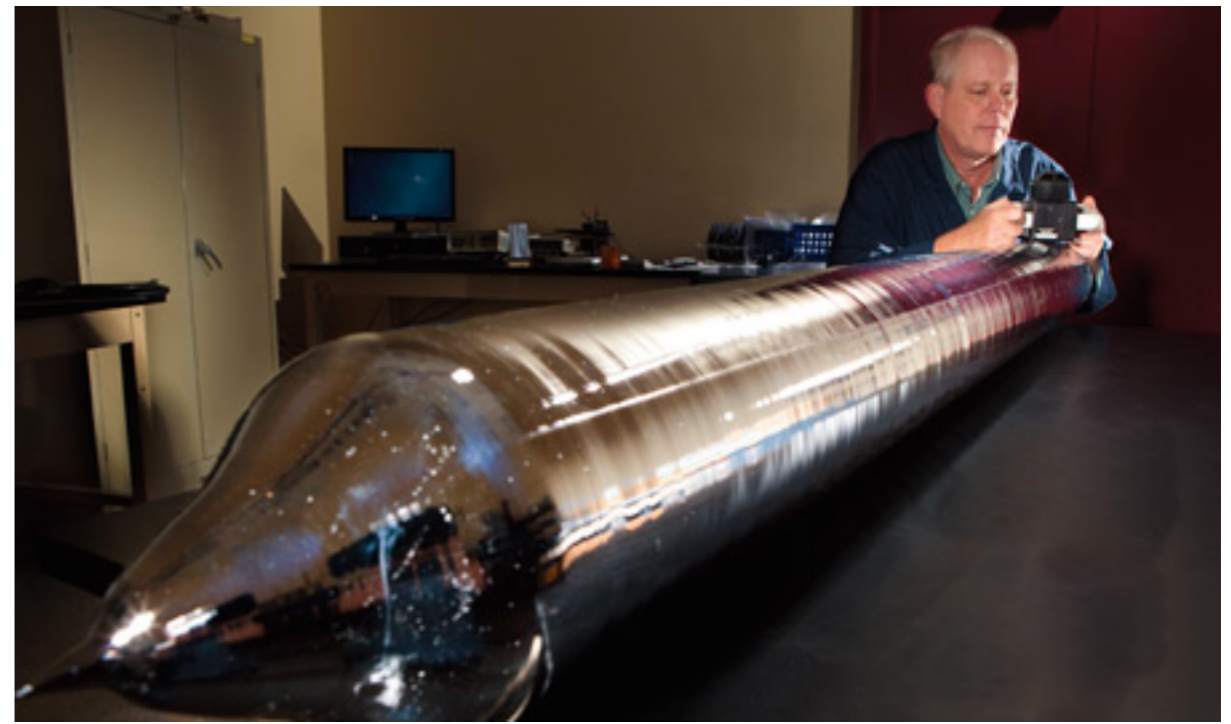


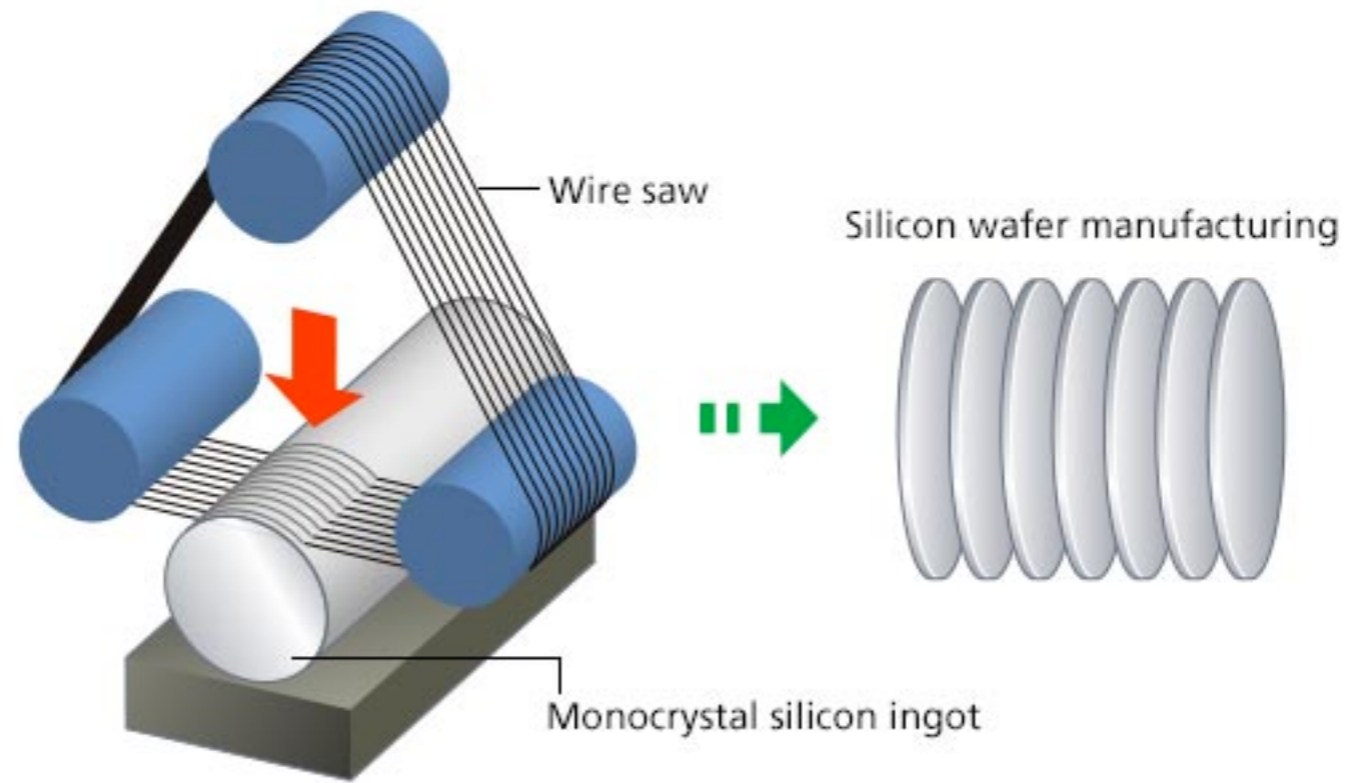
5. Kako gojimo velike kristale? Kako izdelujemo Si waferje?



Czochralski







Preparation of Silicon Wafer

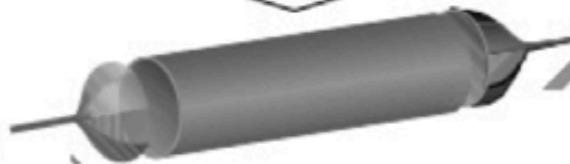
1. Crystal Growth



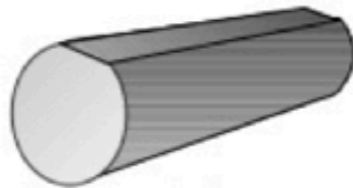
2. Single Crystal Ingot



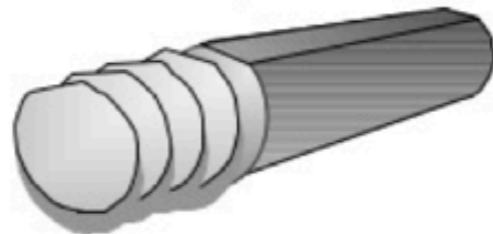
3. Crystal Trimming and Diameter Grind



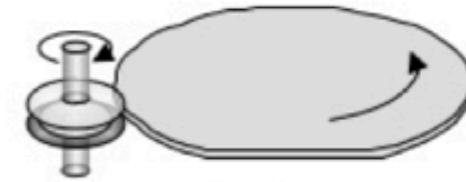
4. Flat Grinding



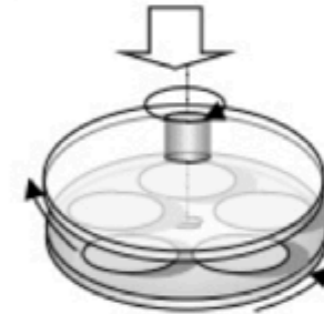
5. Wafer Slicing



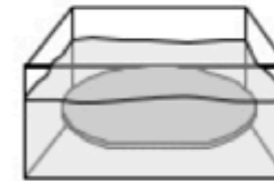
6. Edge Rounding



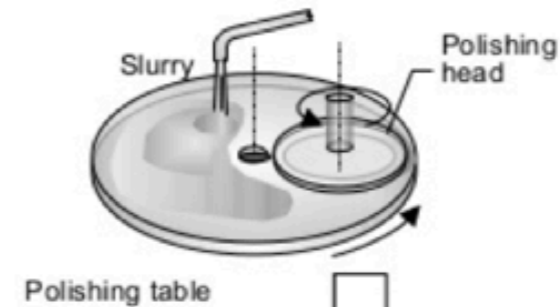
7. Lapping



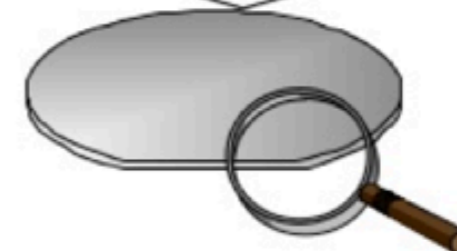
8. Wafer Etching



9. Polishing

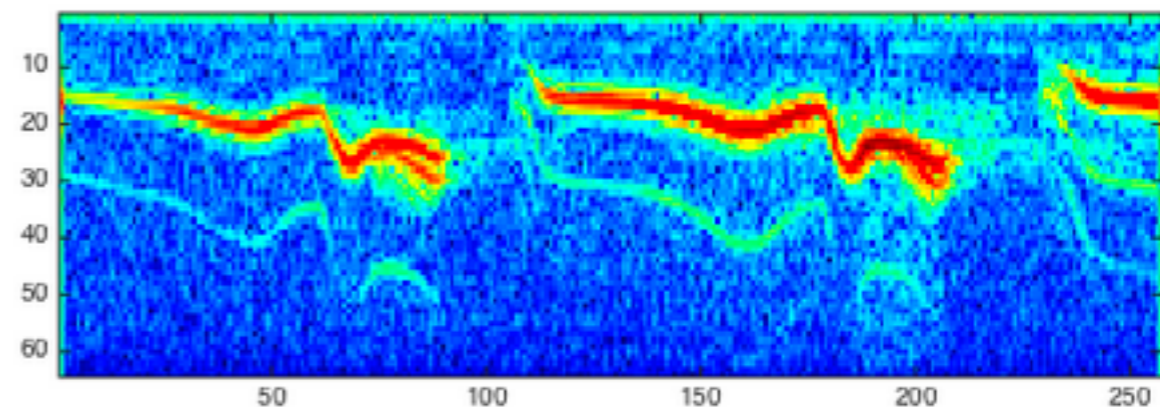
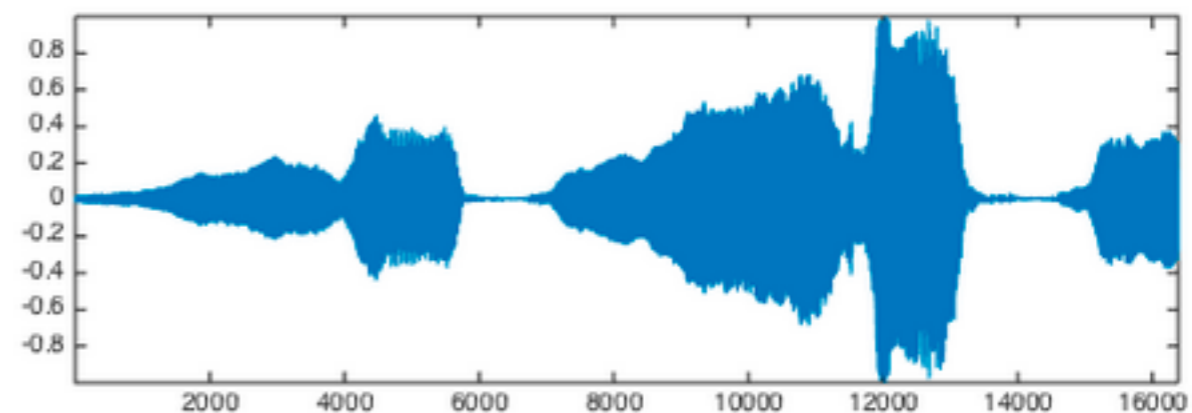
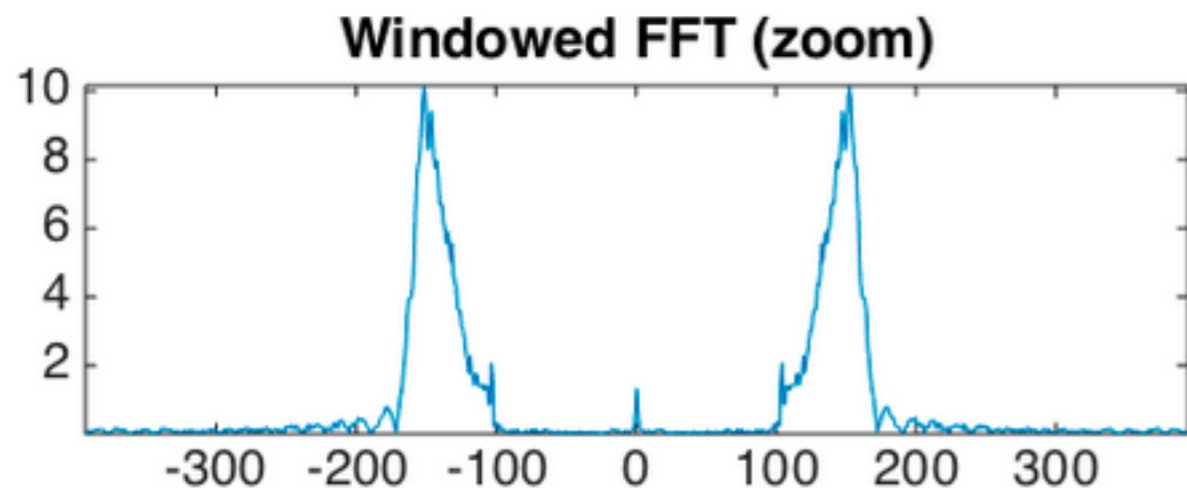
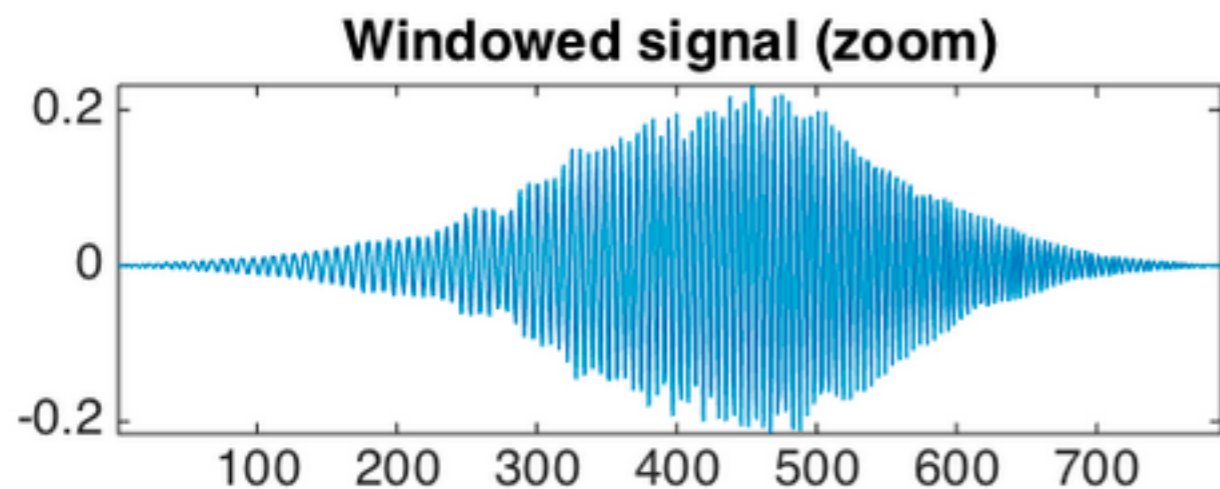


10. Wafer Inspection



6. Kaj je recipročni prostor?

Analogija: zvočni posnetek in spektrogram

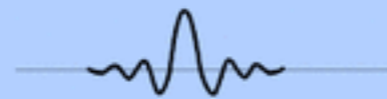


Fourierova transformacija: $\omega \leftrightarrow t$

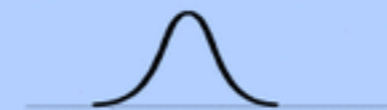
Signal $s(t)$



cosine wave



sinc function



Gaussian



double exponential

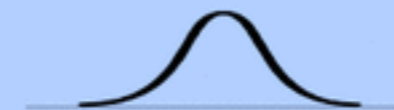
Fourier Transform $S(\omega)$



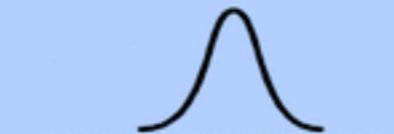
single frequency



uniform band of frequencies



Gaussian

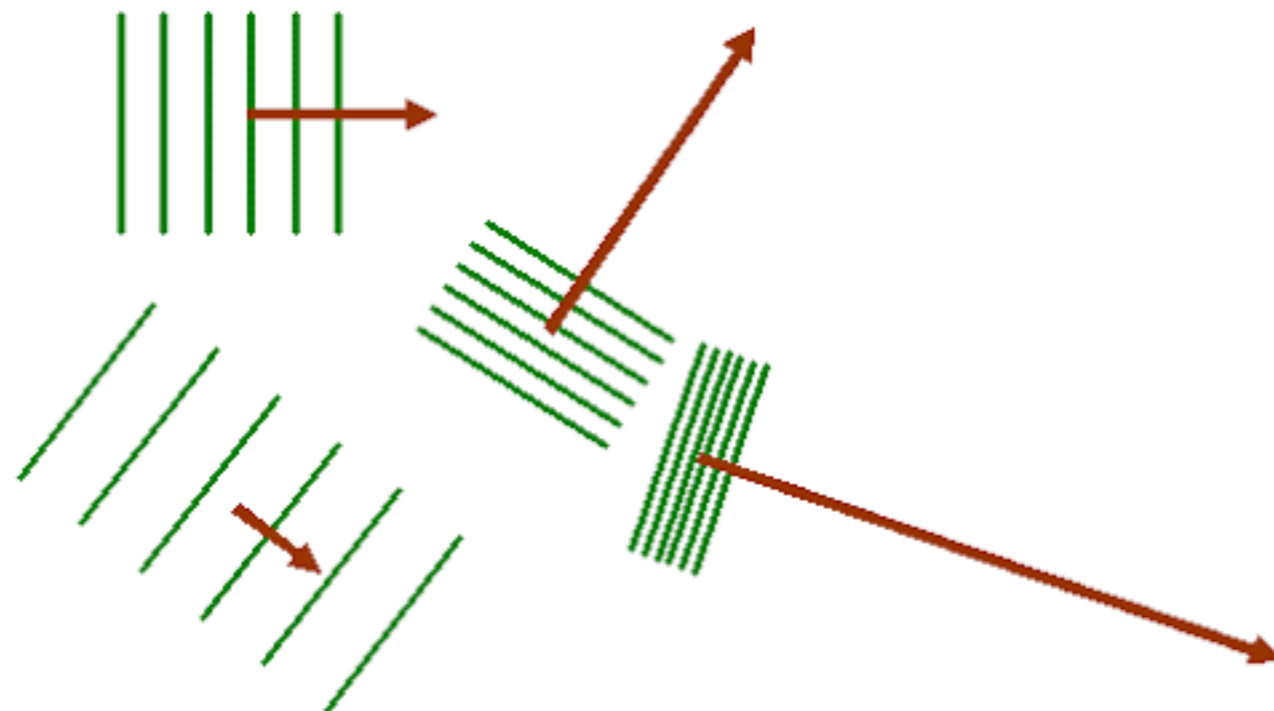


Lorentzian

realni prostor \leftrightarrow reciproční prostor $x \leftrightarrow k$

$$\hat{f}(k) = \int f(x) e^{-ik \cdot x} dx$$

$$f(x) = \frac{1}{(2\pi)^d} \int \hat{f}(k) e^{ik \cdot x} dk$$

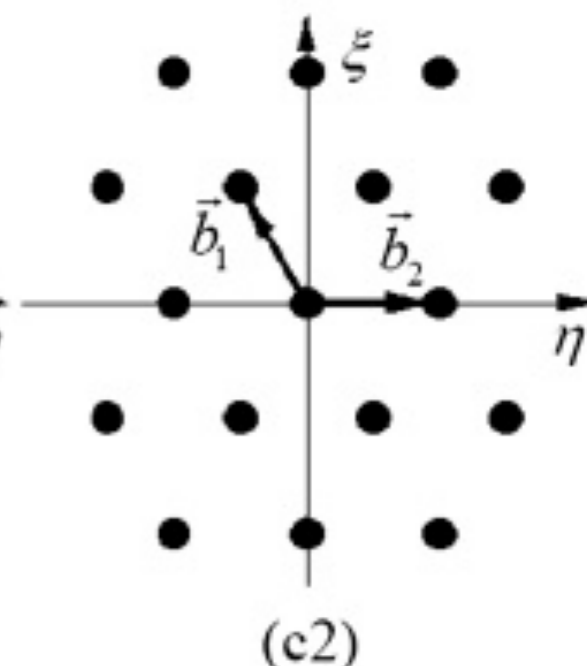
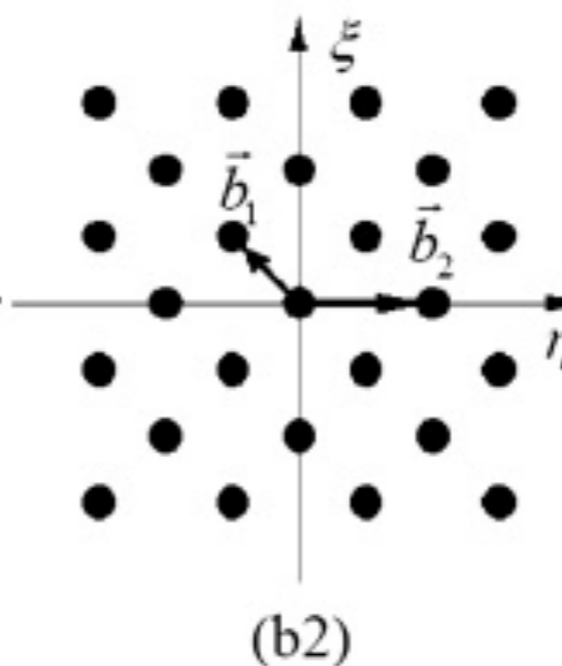
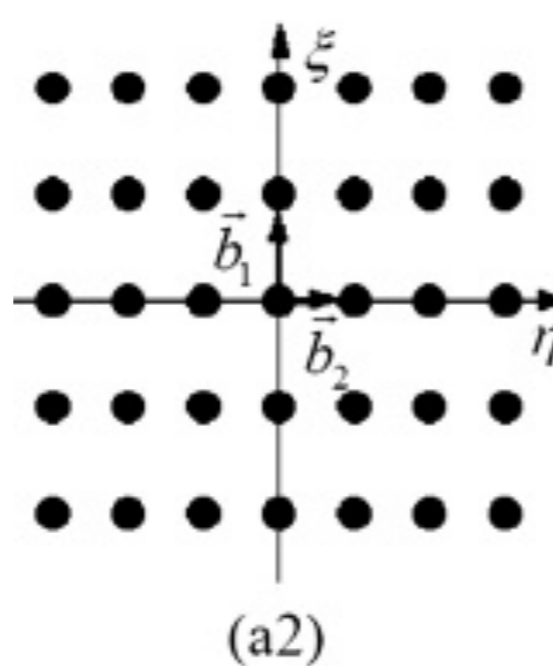
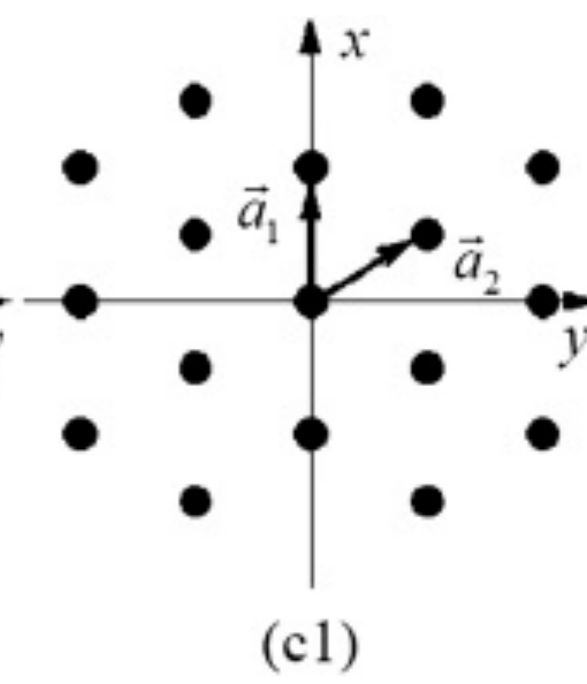
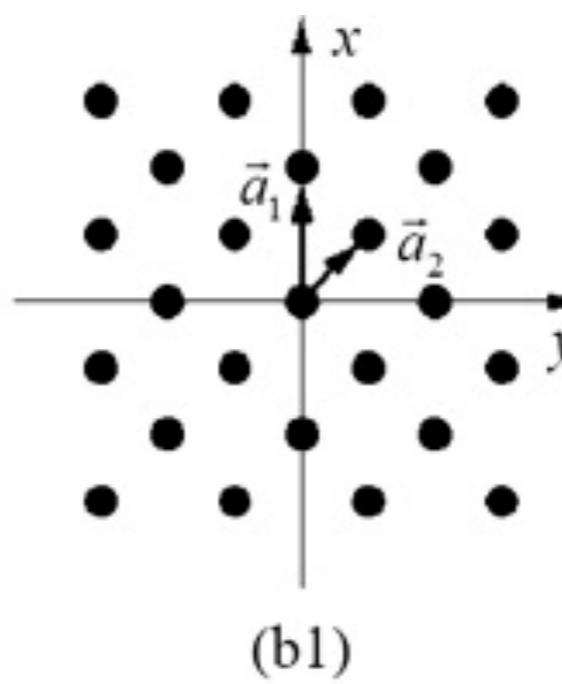
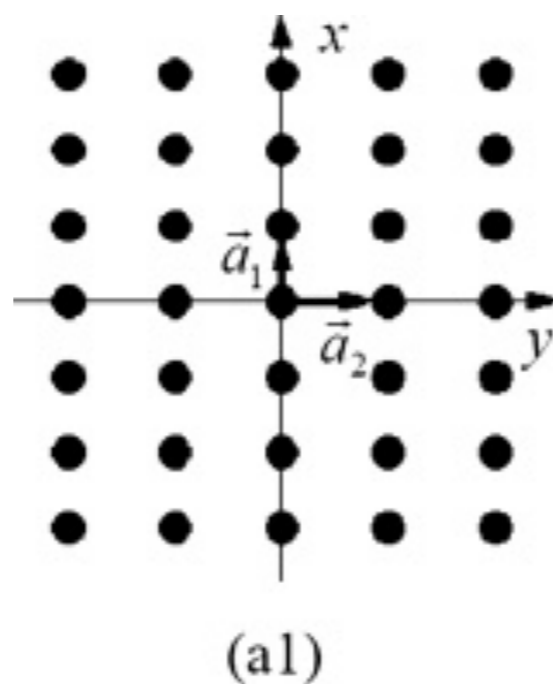


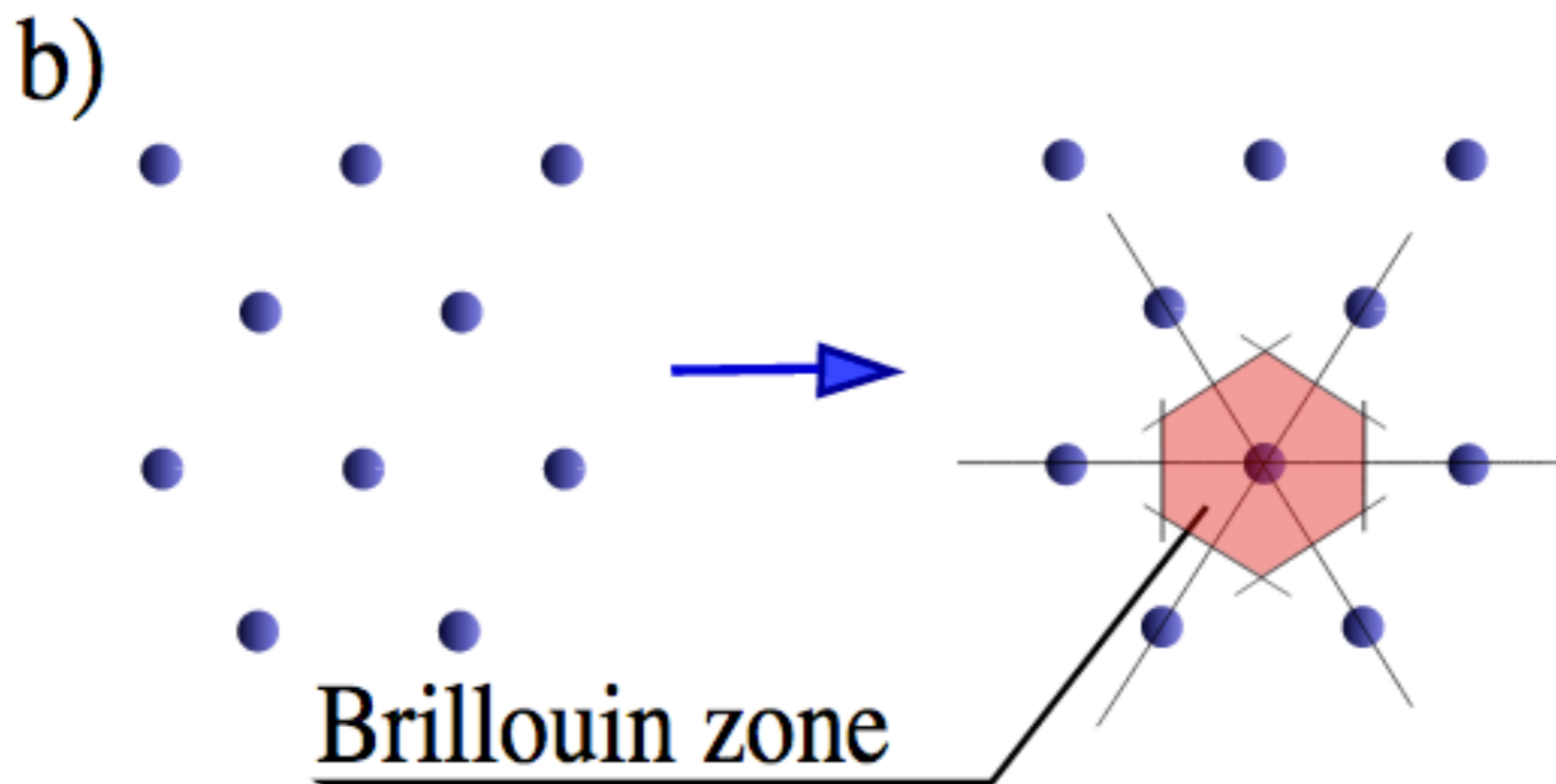
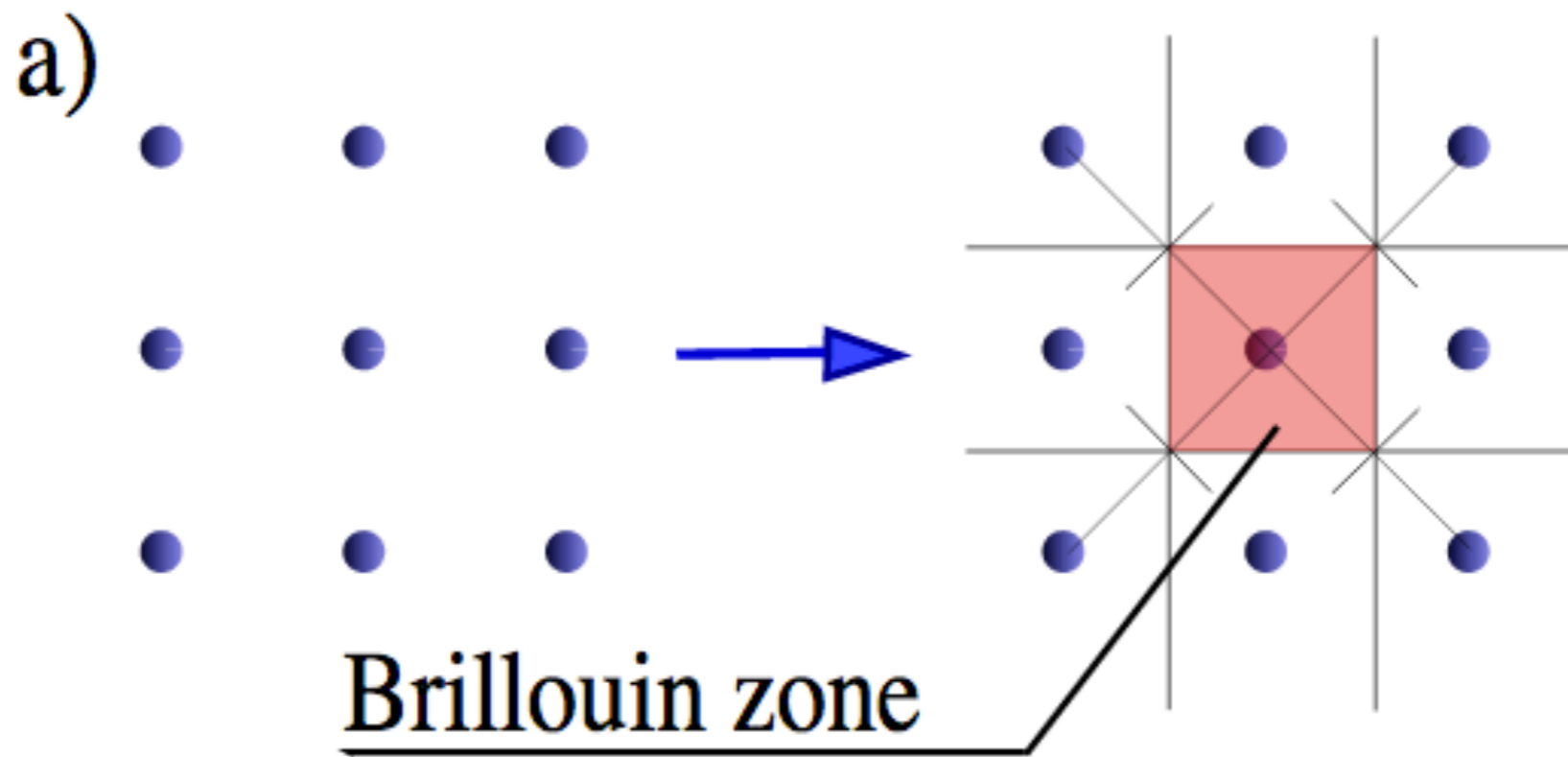
RECIPROČNI MREŽA

$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{V_{\text{celica}}}$$

$$\mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{V_{\text{celica}}}$$

$$\mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{V_{\text{celica}}}$$



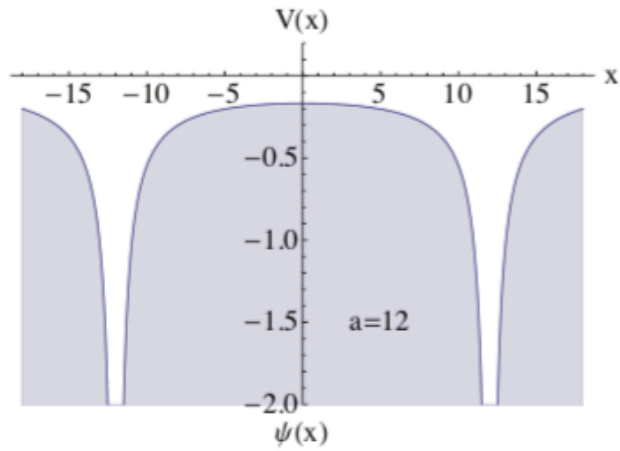


7. Kaj je elektronski pas?

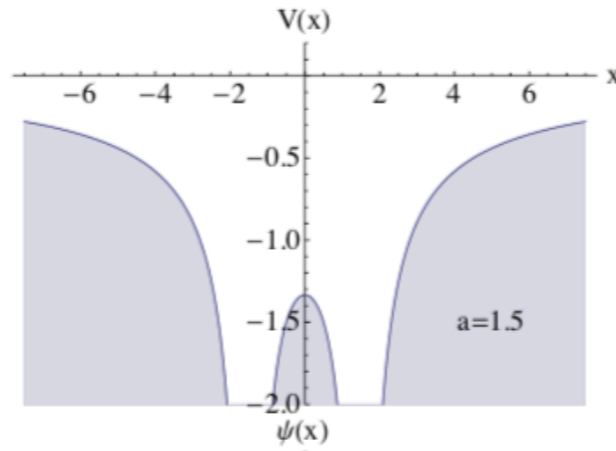
V čem se razlikujejo kovine in izolatorji?

N=2

večja oddaljenost med jedroma

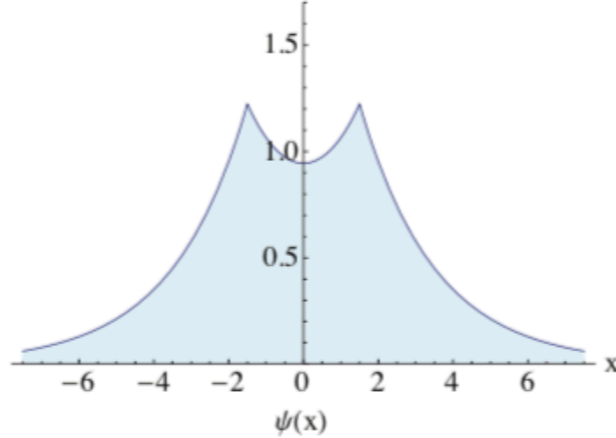
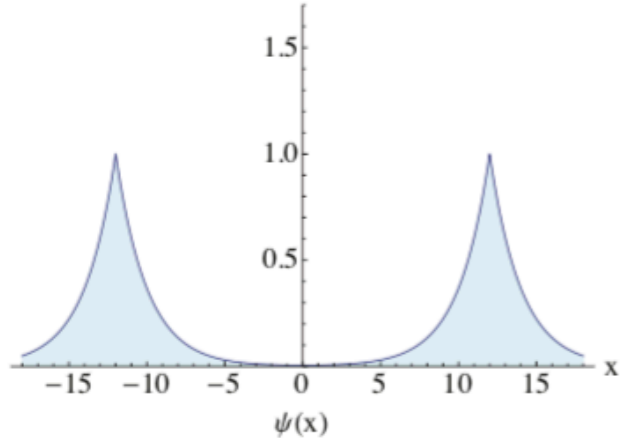


manjša oddaljenost med jedroma

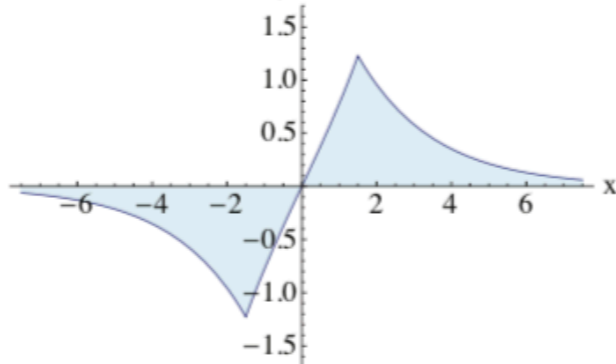
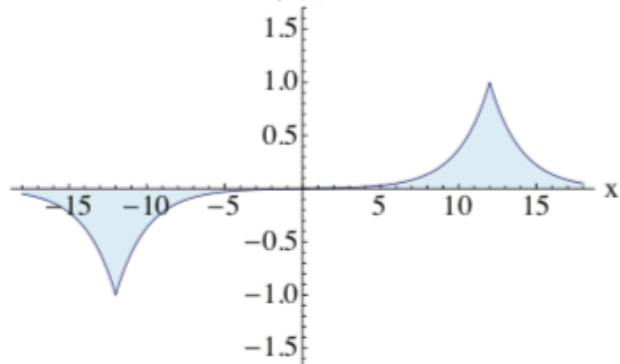


$$\psi_{\text{soda}}(\mathbf{r}) = \frac{1}{\sqrt{2}} [\psi(\mathbf{r} - \mathbf{r}_A) + \psi(\mathbf{r} - \mathbf{r}_B)]$$

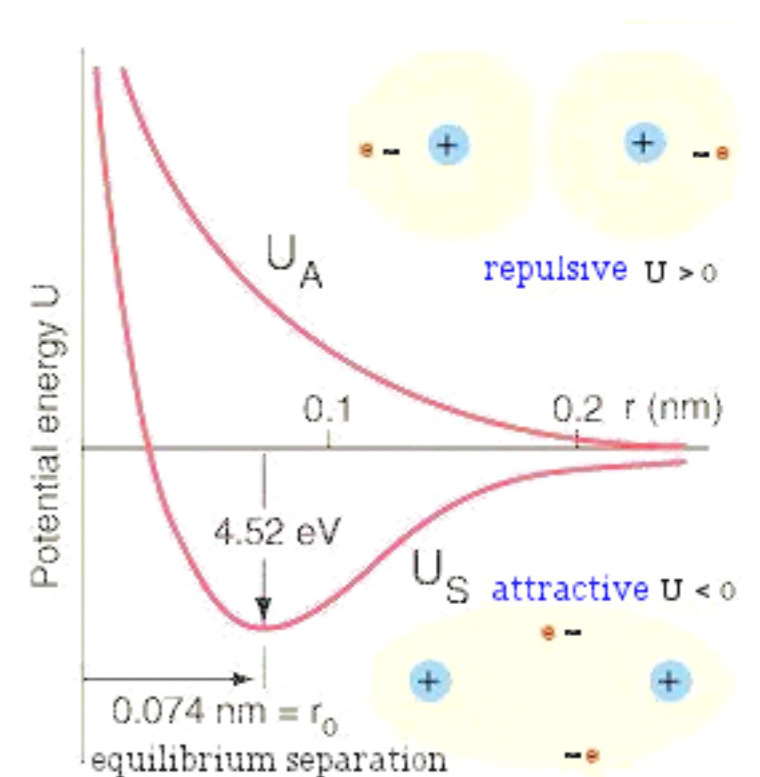
$$\psi_{\text{liha}}(\mathbf{r}) = \frac{1}{\sqrt{2}} [\psi(\mathbf{r} - \mathbf{r}_A) - \psi(\mathbf{r} - \mathbf{r}_B)]$$



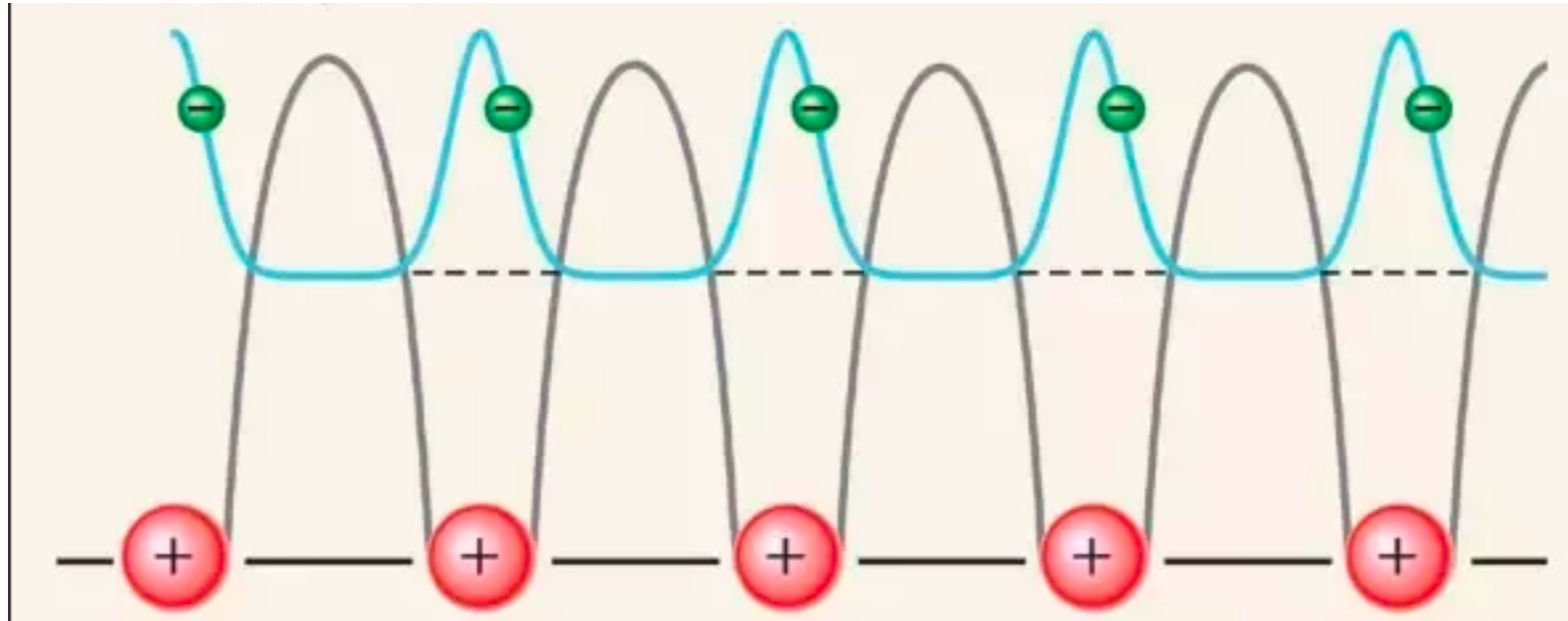
soda kombinacija



liha kombinacija



N velik



$$H = \sum_j \epsilon |j\rangle \langle j| - t (|j\rangle \langle j+1| + |j\rangle \langle j-1|)$$

$$H = \begin{pmatrix} \epsilon & -t & 0 & 0 & \dots & 0 \\ -t & \epsilon & -t & 0 & \dots & 0 \\ 0 & -t & \epsilon & -t & \dots & 0 \\ 0 & 0 & -t & \epsilon & -t & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & \dots & \dots & \epsilon & -t \\ 0 & \dots & \dots & \dots & -t & \epsilon \end{pmatrix}$$

$$|\psi_k\rangle = \sum_j e^{ikja} |j\rangle$$

$$H = \sum_j \epsilon |j\rangle \langle j| - t (|j\rangle \langle j+1| + |j\rangle \langle j-1|)$$

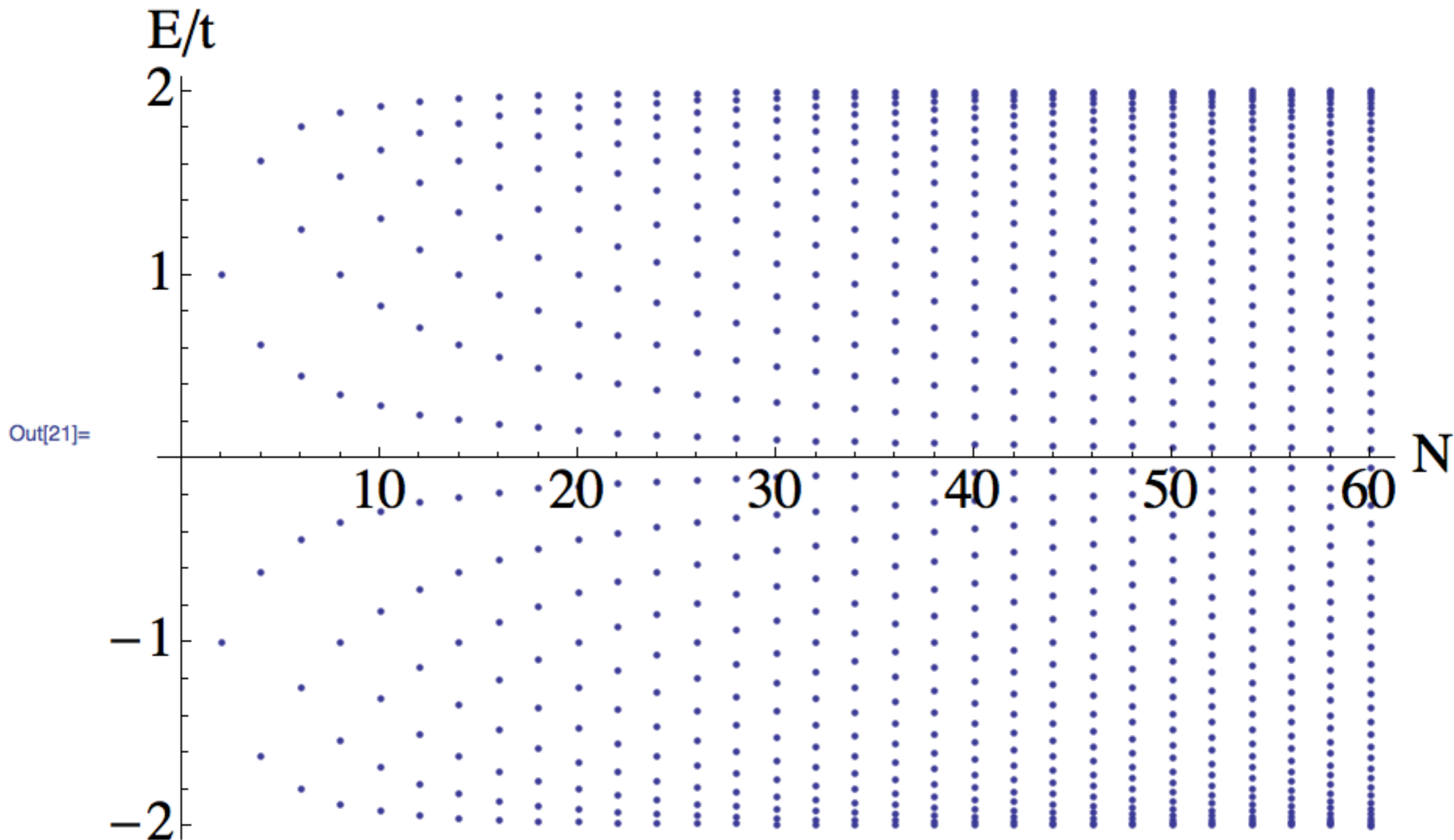
$$|\psi_k\rangle = \sum_j e^{ikja} |j\rangle$$

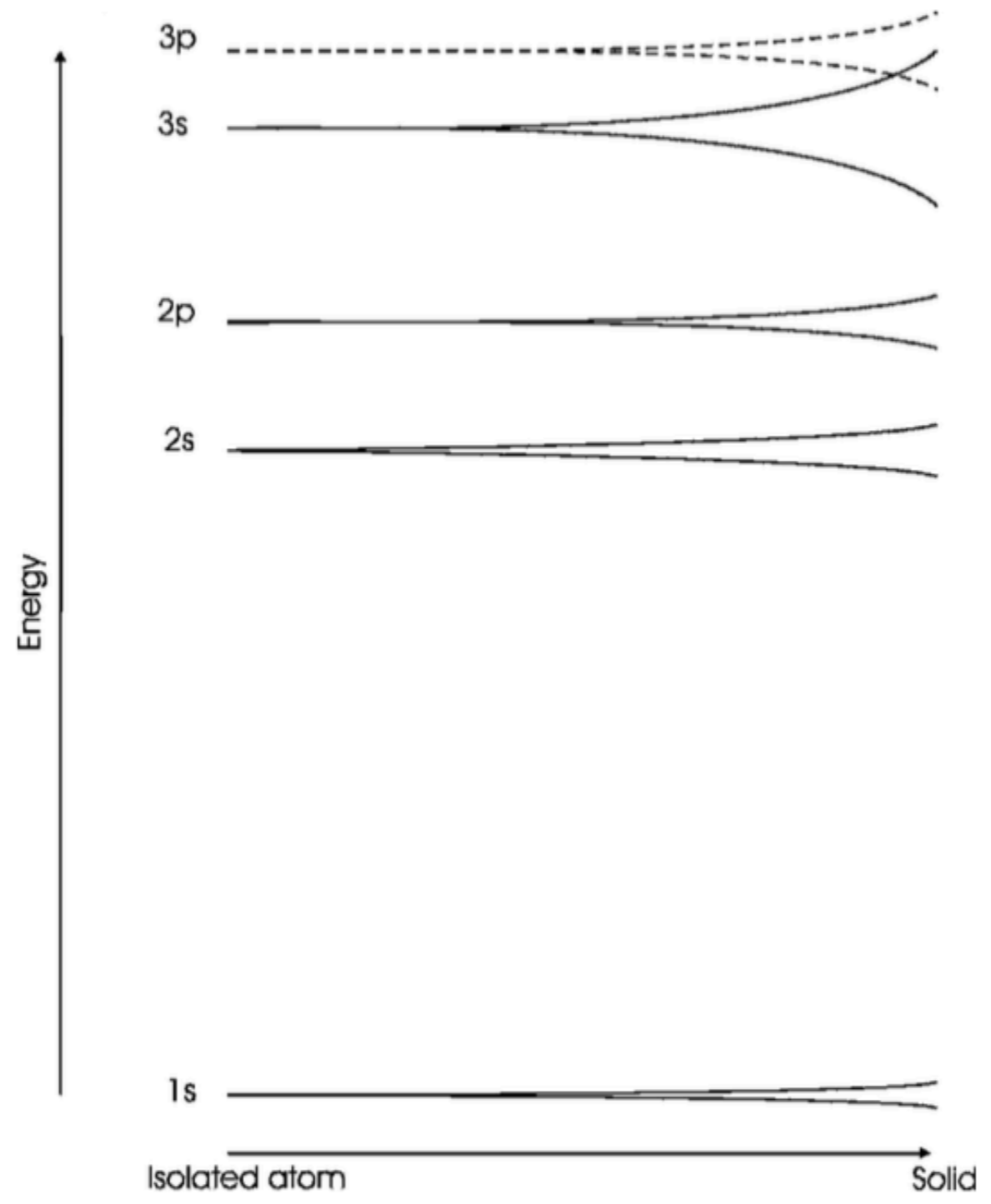
$$\begin{aligned} H |\psi_k\rangle &= \sum_j e^{ikja} \epsilon |j\rangle - t e^{ikja} (e^{ika} |j\rangle + e^{-ika} |j\rangle) \\ &= \sum_j [\epsilon - 2t \cos(ka)] e^{ikja} |j\rangle \\ &= [\epsilon - 2t \cos(ka)] |\psi_k\rangle . \end{aligned}$$

$$E(k) = \epsilon - 2t \cos(ka).$$

$$E(k) = \epsilon - 2t \cos(ka)$$

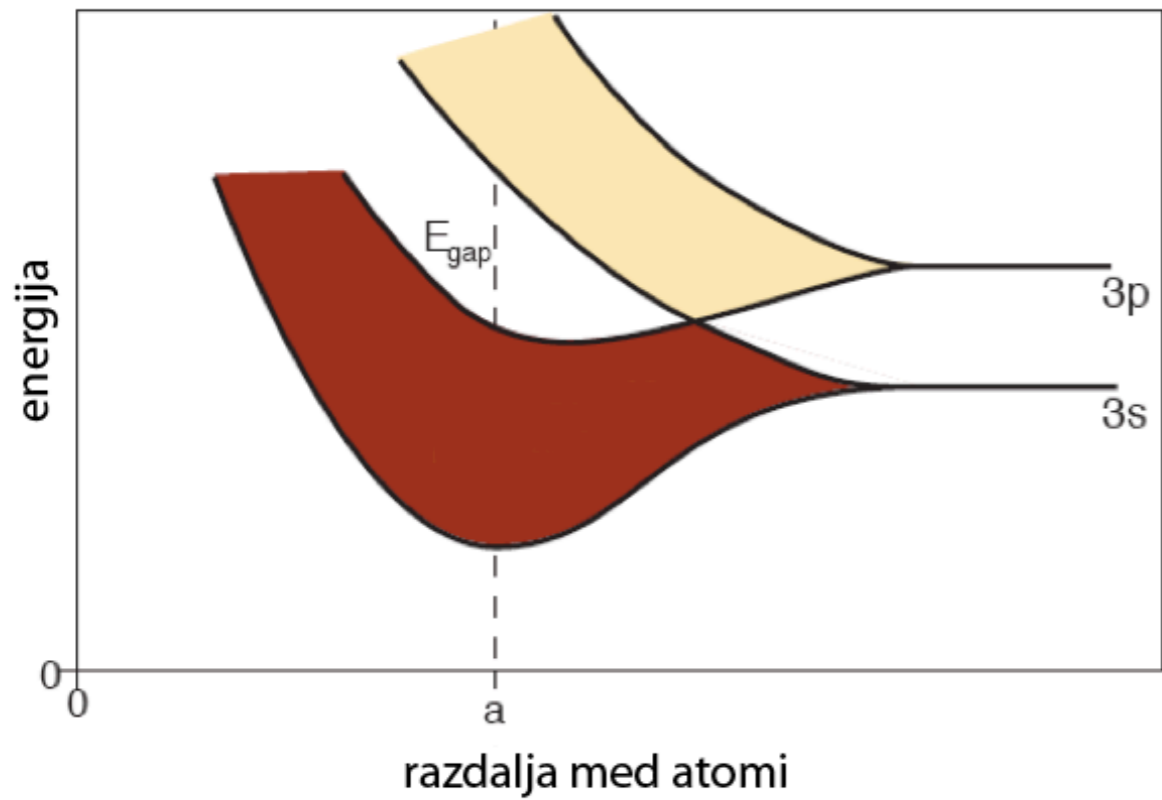
```
In[20]:= l = Flatten[Table[Table[{nn, -2 Cos[n Pi / (nn + 1)]}, {n, 1, nn}], {nn, 2, 60, 2}], 1];  
ListPlot[l, AxesLabel -> {"N (sod)", "E/t"}, AxesStyle -> Large, ImageSize -> 8 x 72]
```



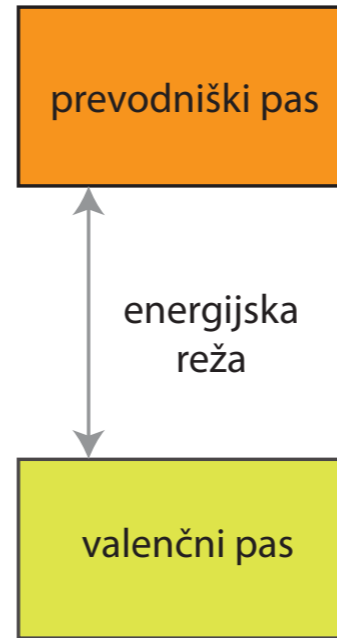


Mg

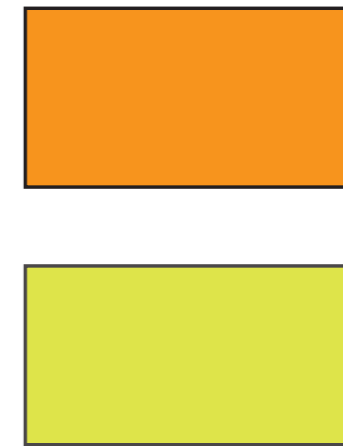
TEORIJA PASOV



energija stanj



izolator

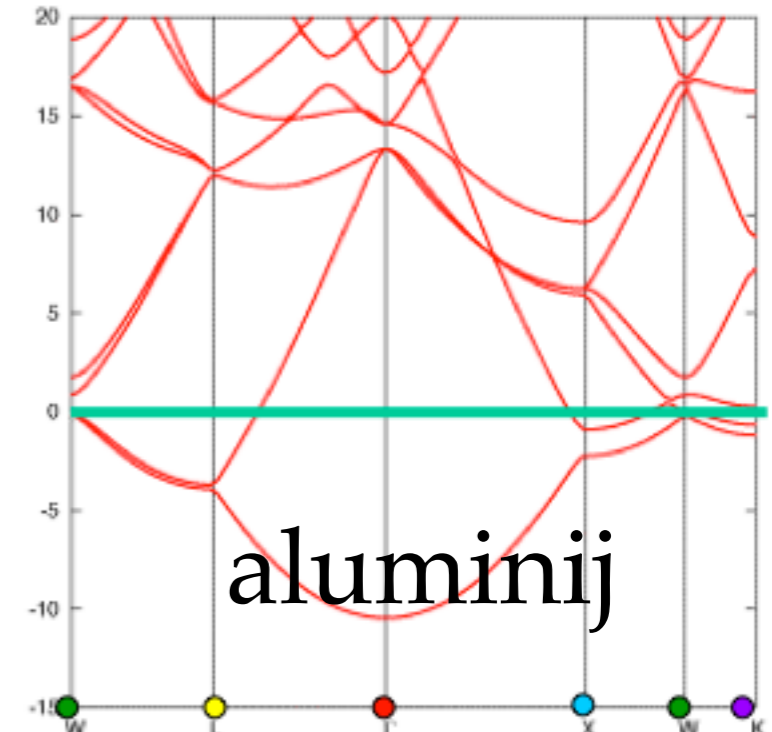
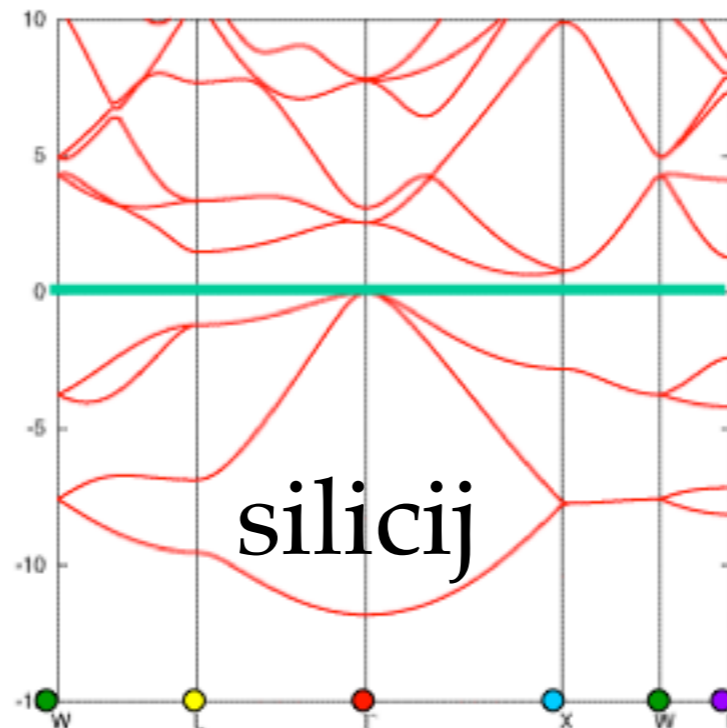
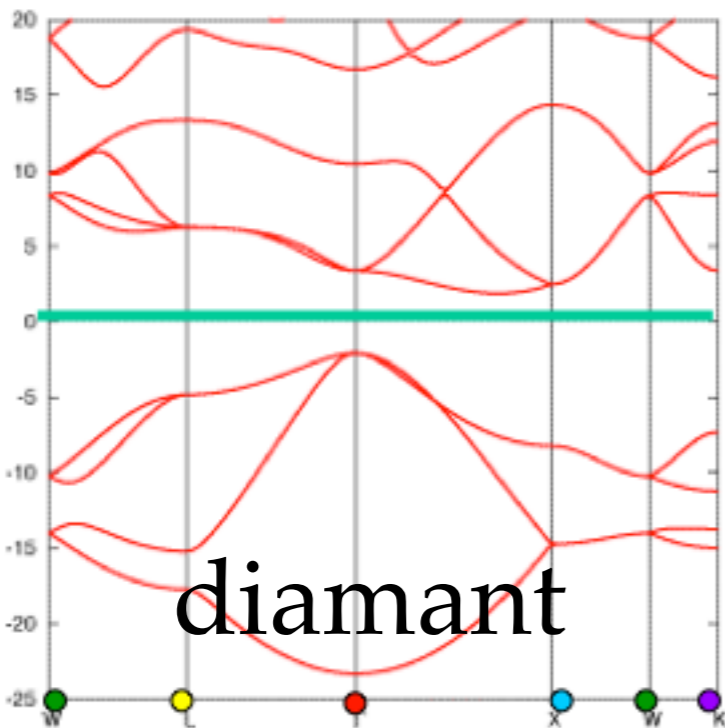
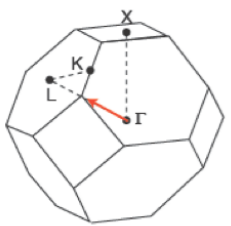


polprevodnik

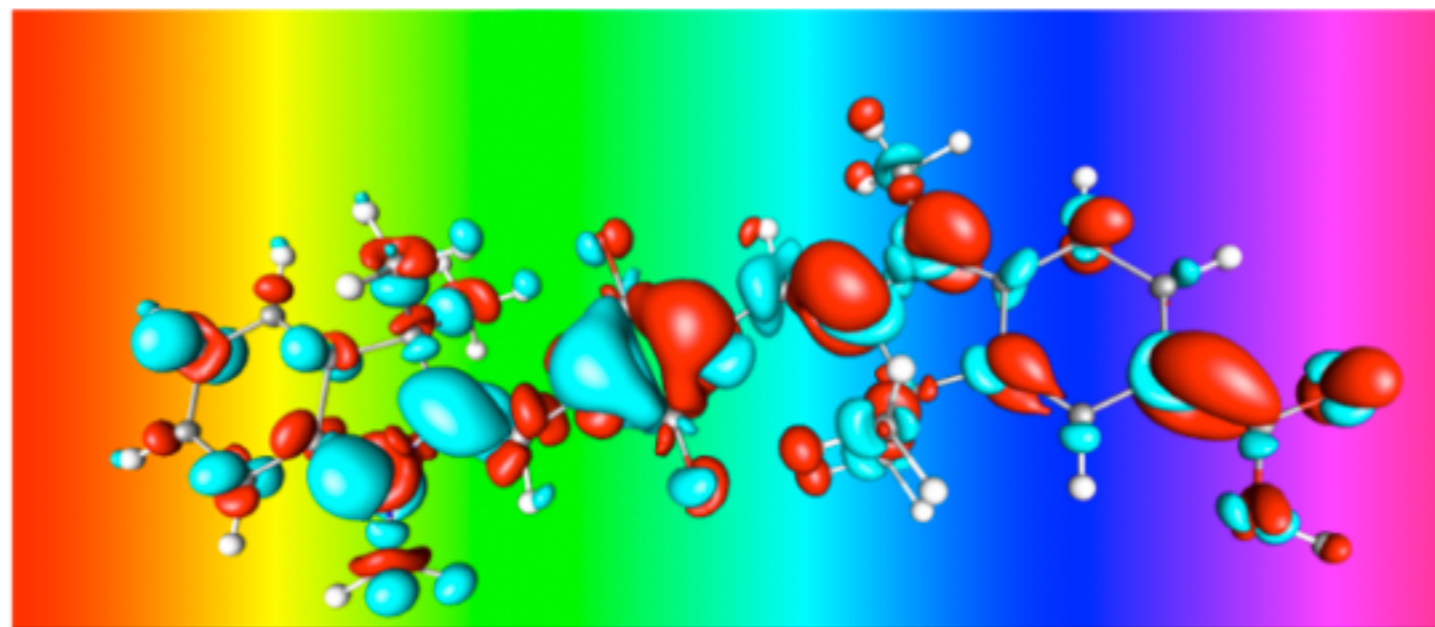


kovina

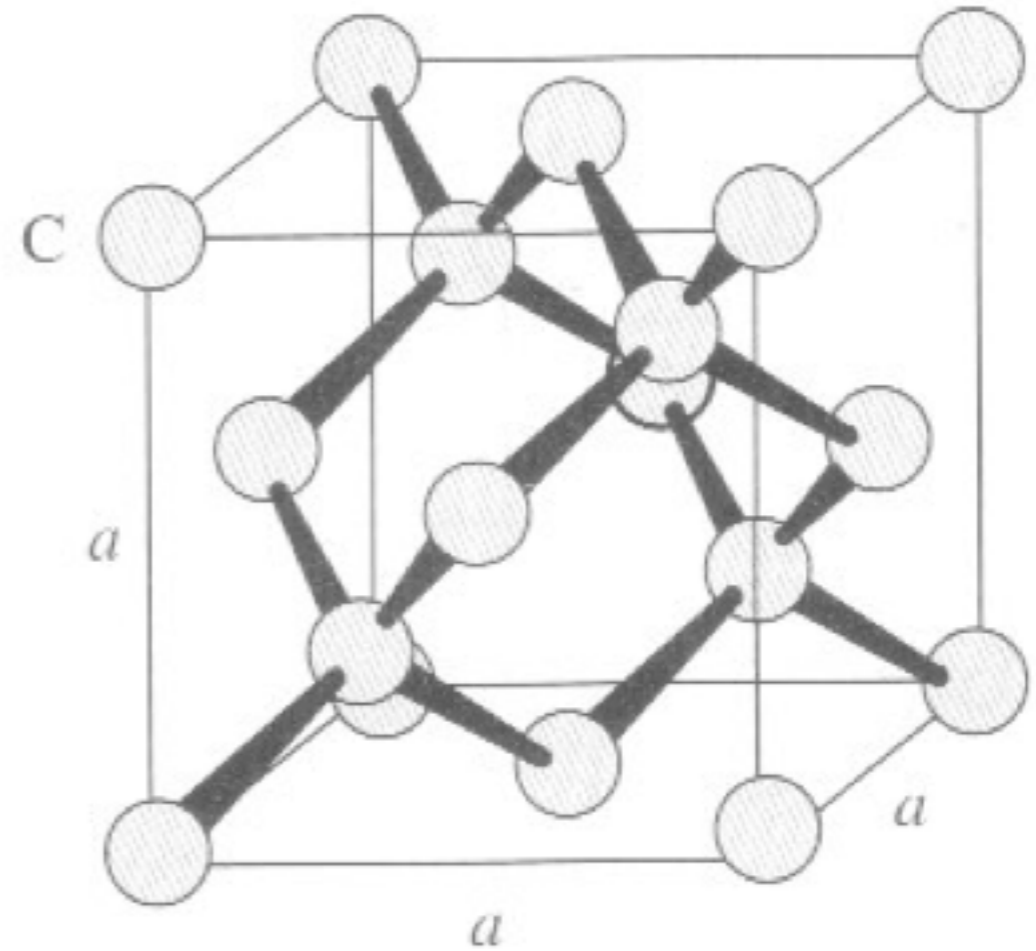
pasovna
struktura

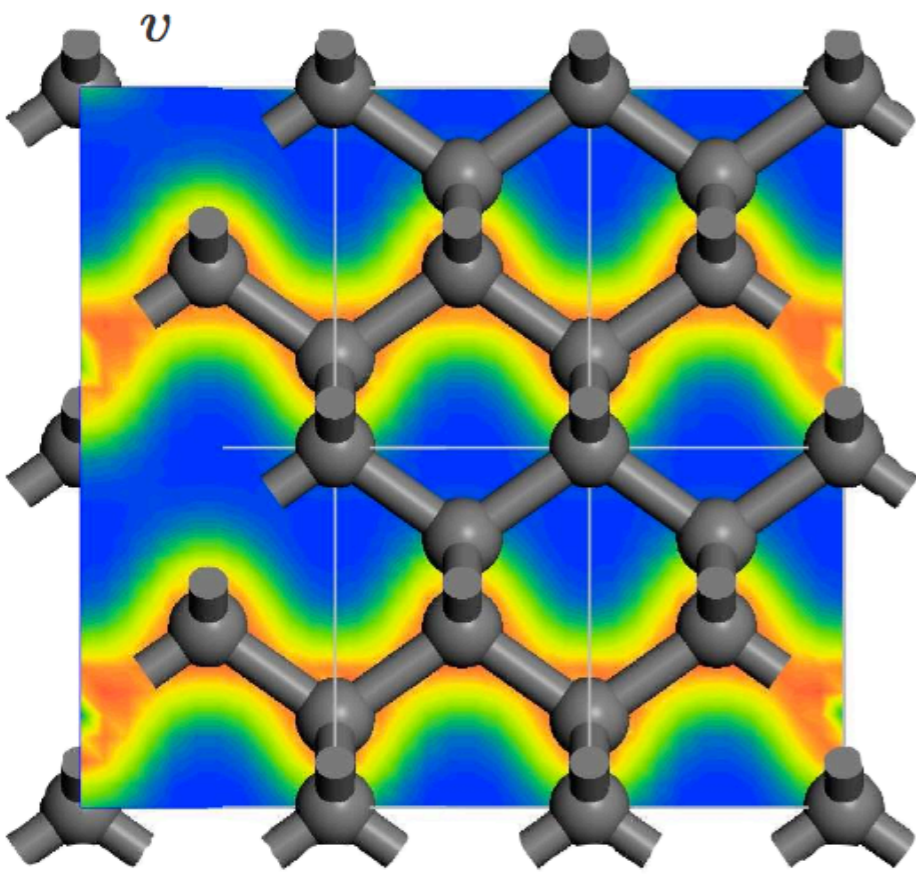


Računska kemija

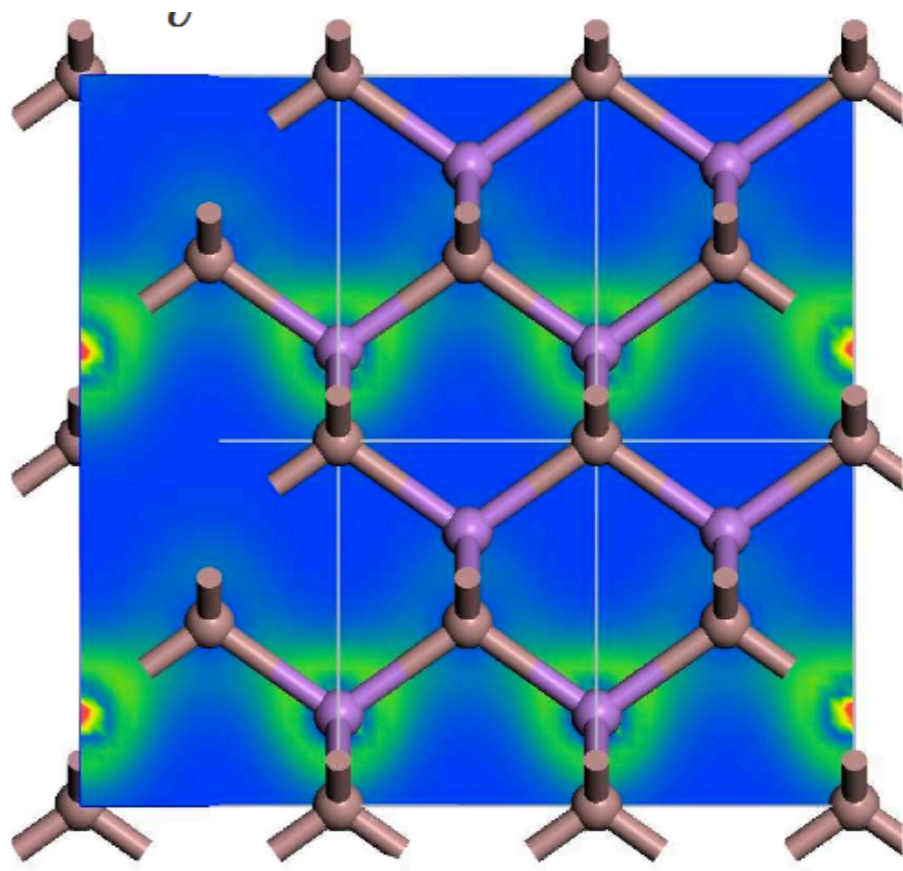


```
&control
  calculation = 'scf',
  prefix = 'Si_exc1',
/
&system
 ibrav = 2,
  celldm(1) = 10.26,
  nat = 2,
  ntyp = 1,
  ecutwfc = 20
/
&electrons
  mixing_beta = 0.7
/
ATOMIC_SPECIES
Si 28.086 Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
Si 0.0 0.0 0.0
Si 0.25 0.25 0.25
K_POINTS (automatic)
6 6 6 1 1 1
```

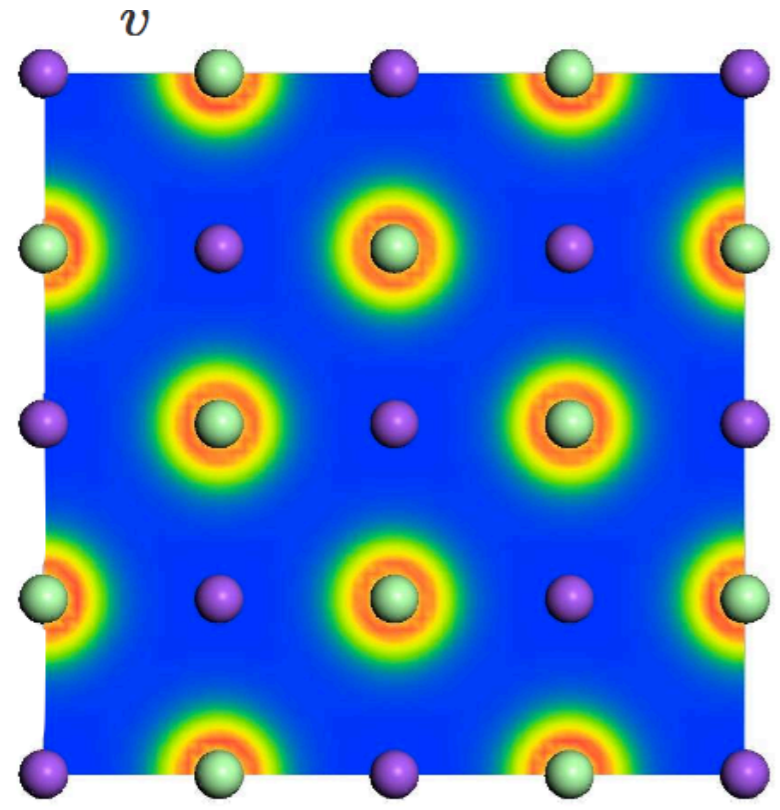




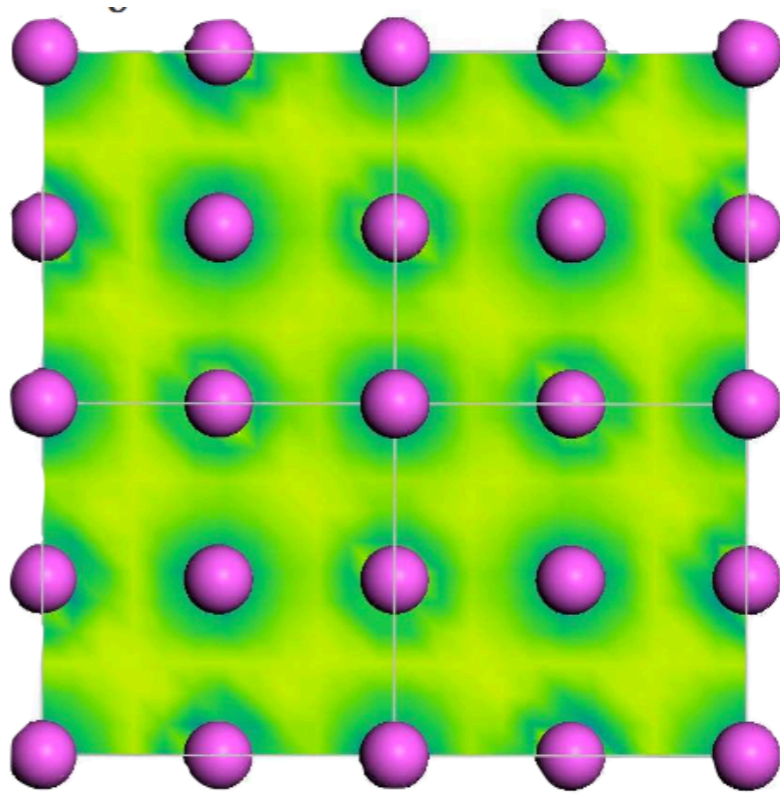
diamond



GaAs

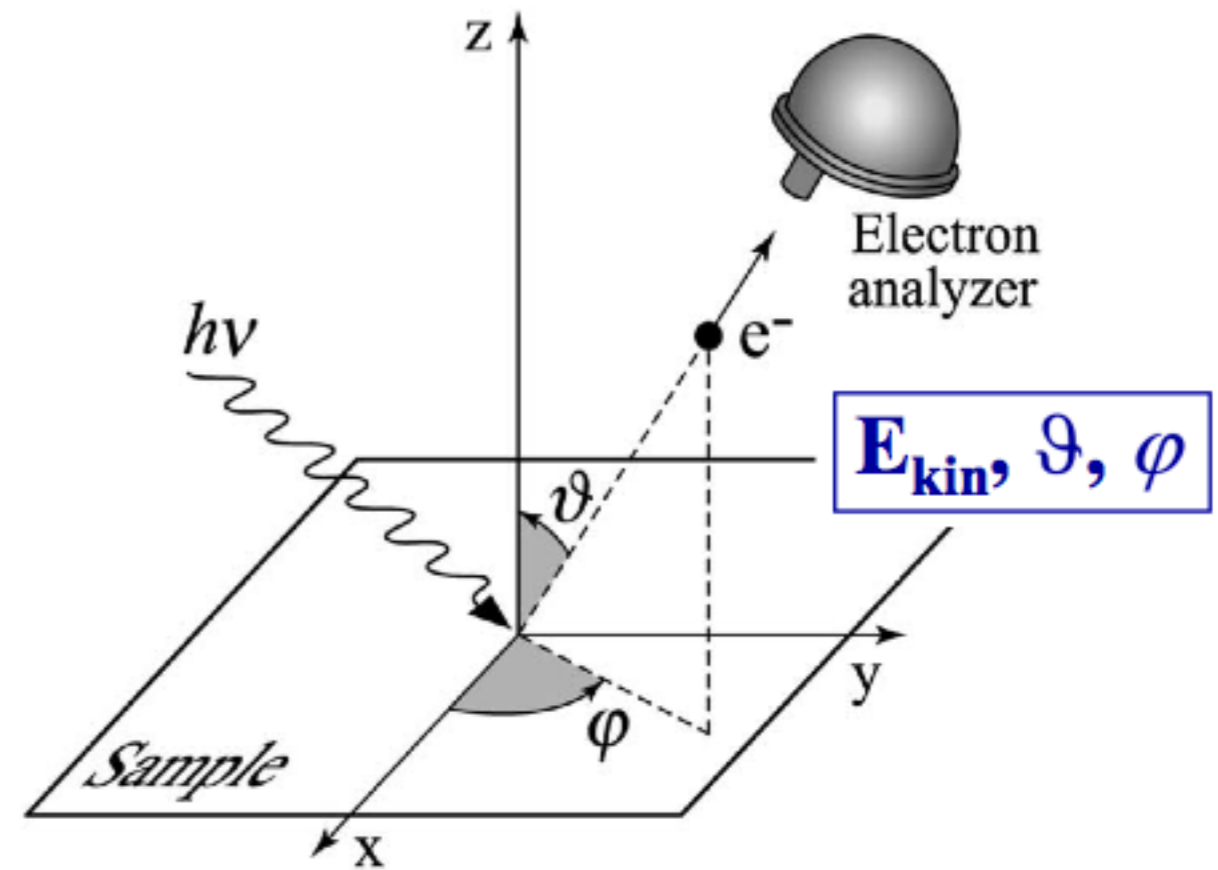
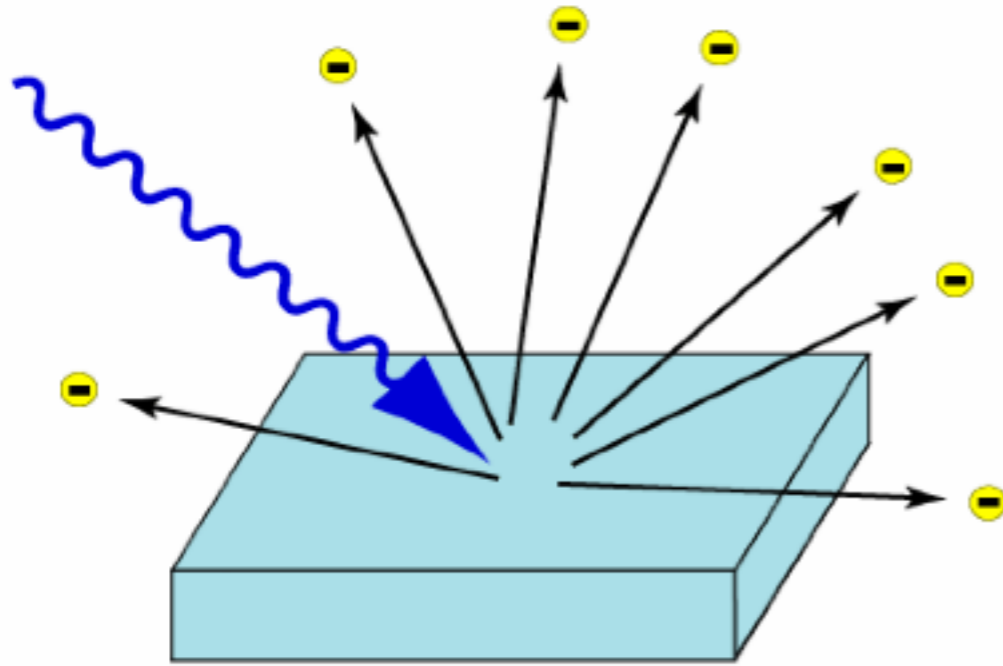


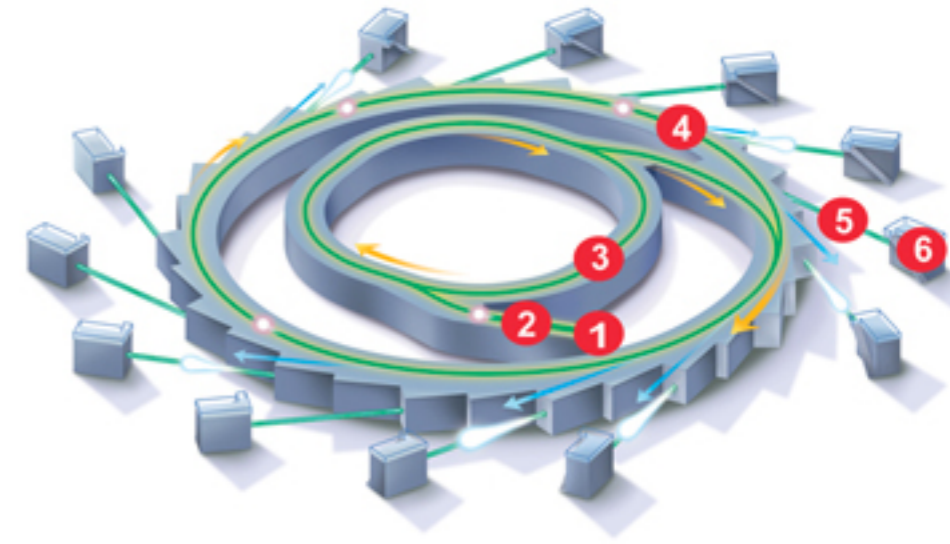
NaCl



Aluminum

ARPES





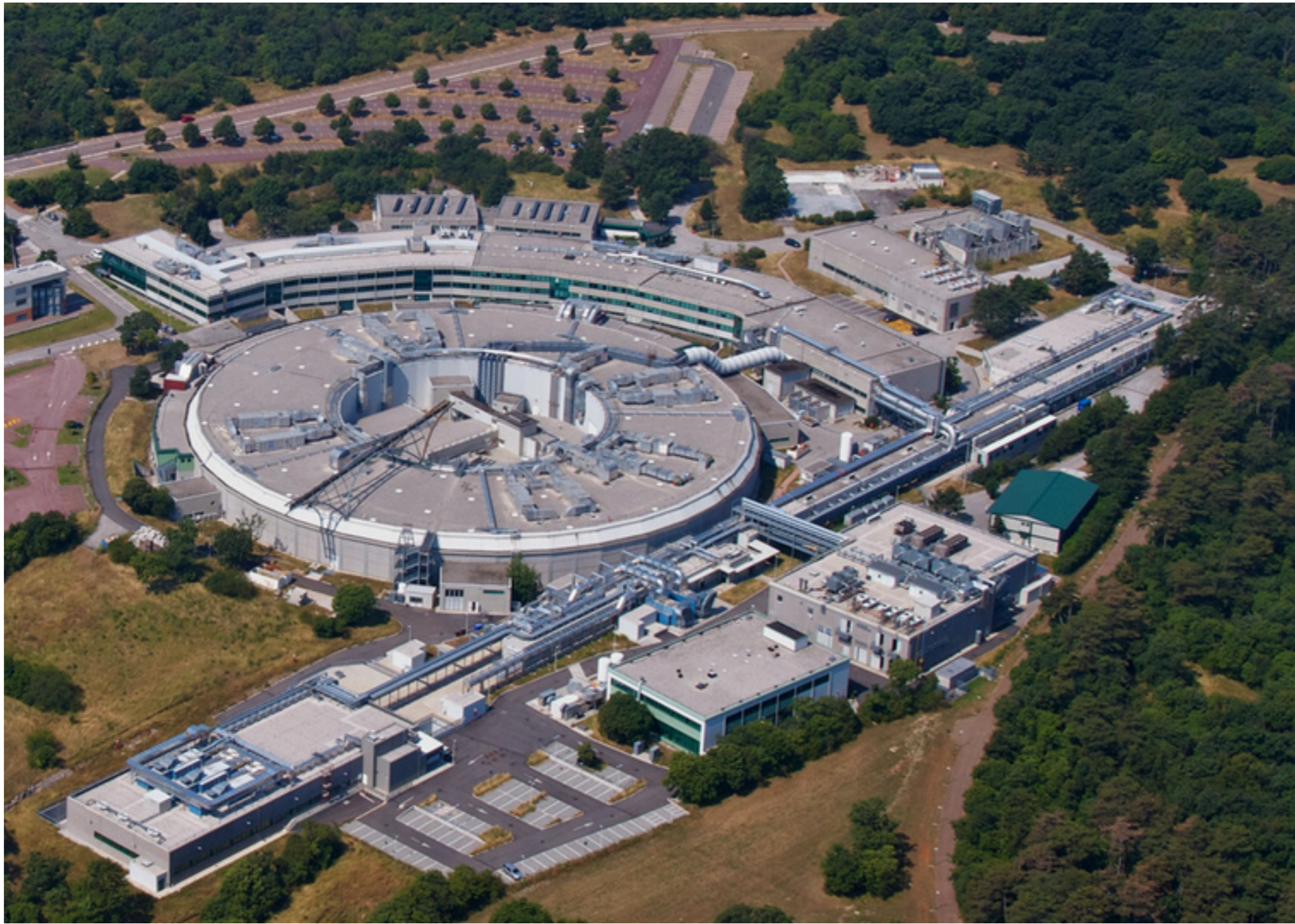
Diamond (UK, blizu Oxforda)

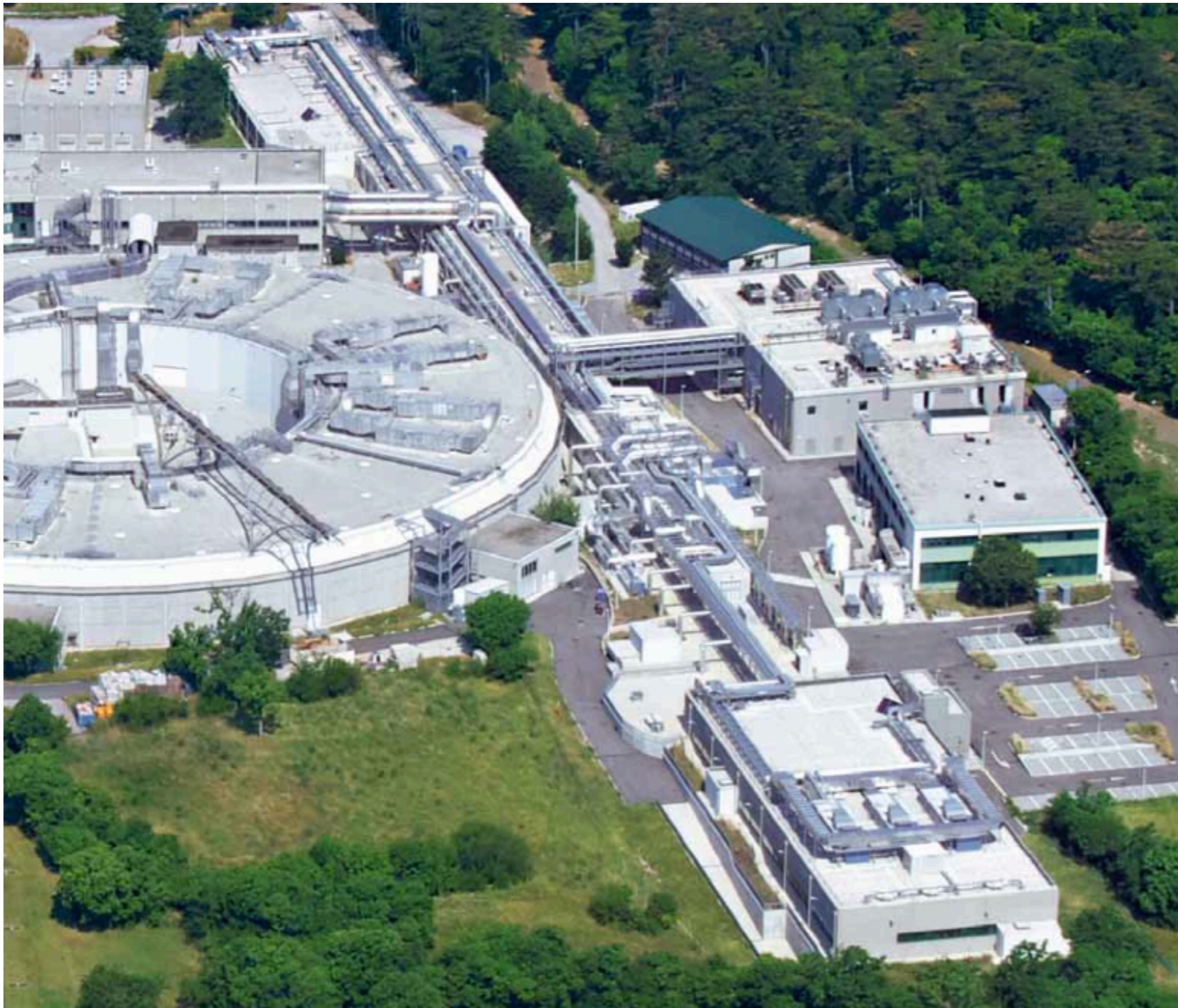


Peking (2018)



Elettra, Bazovica





Elettra, Bazovica pri Trstu

