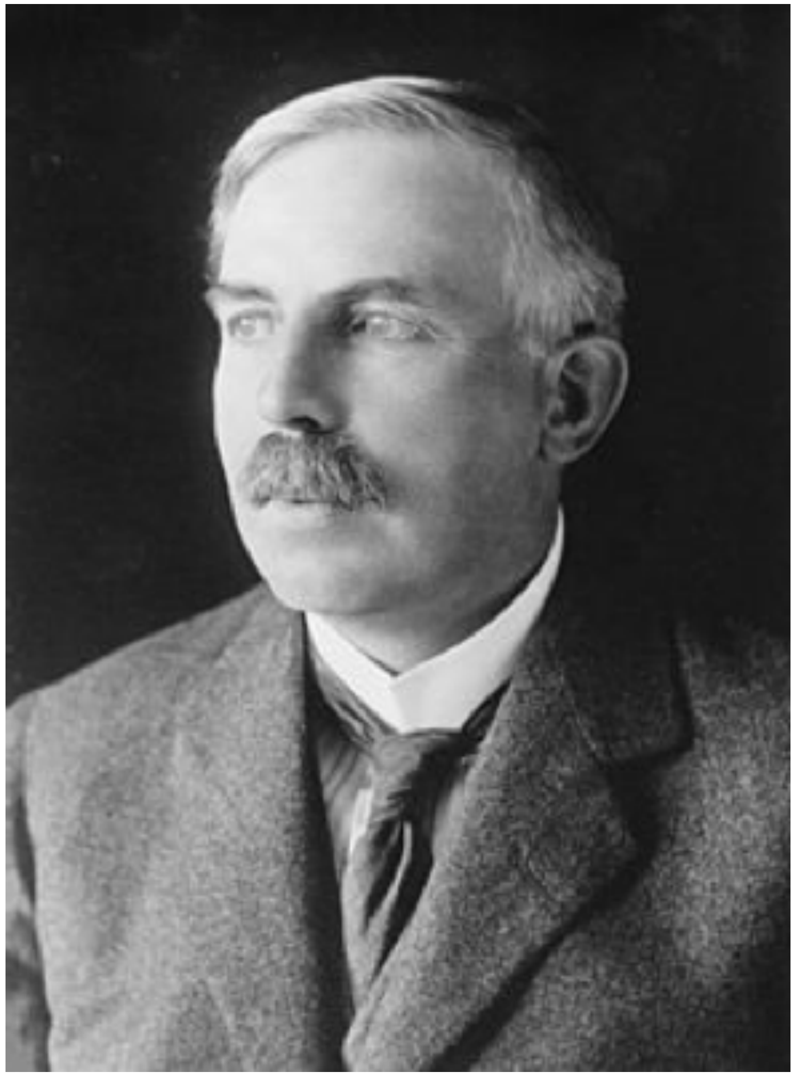
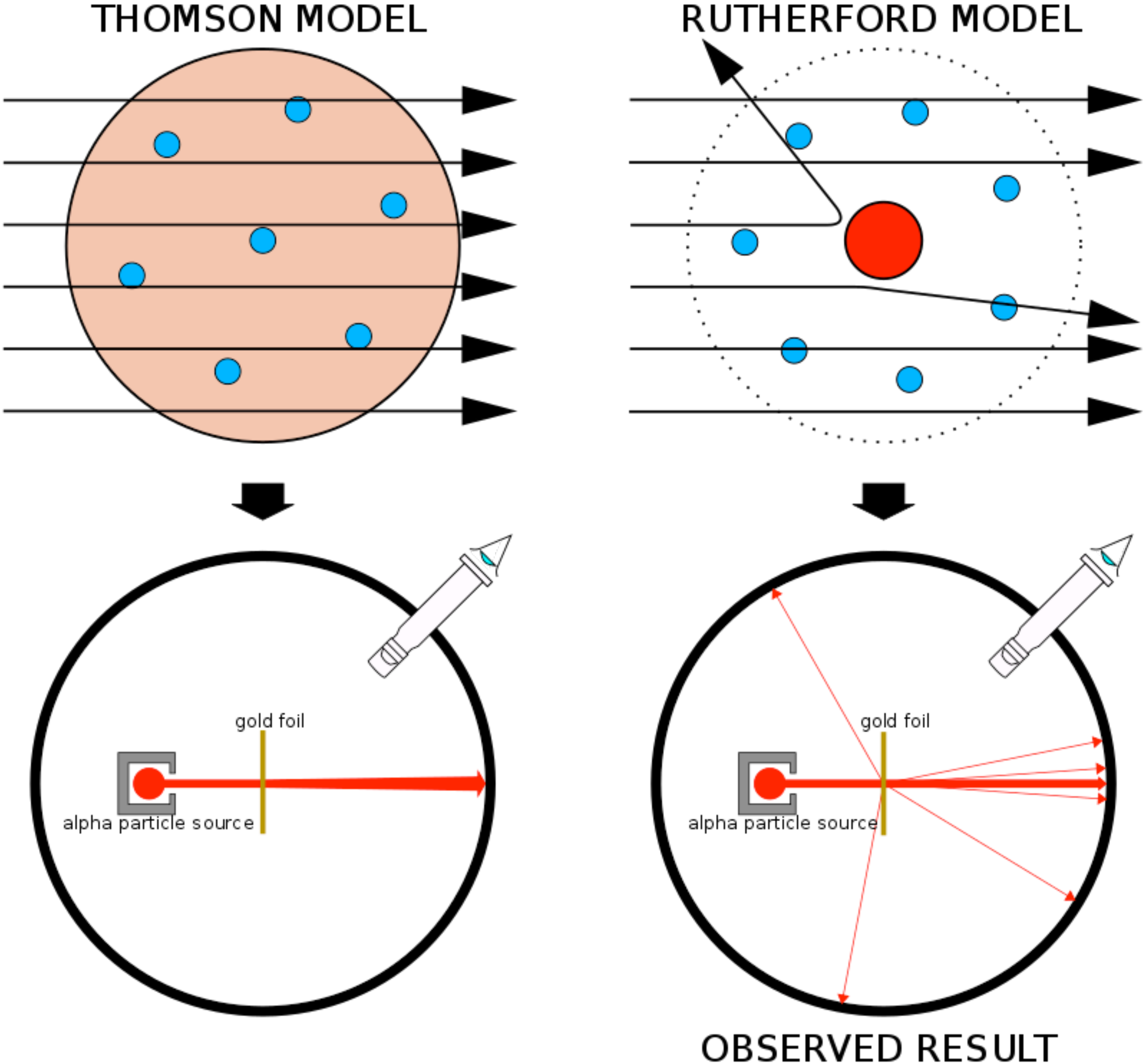


Rutherford

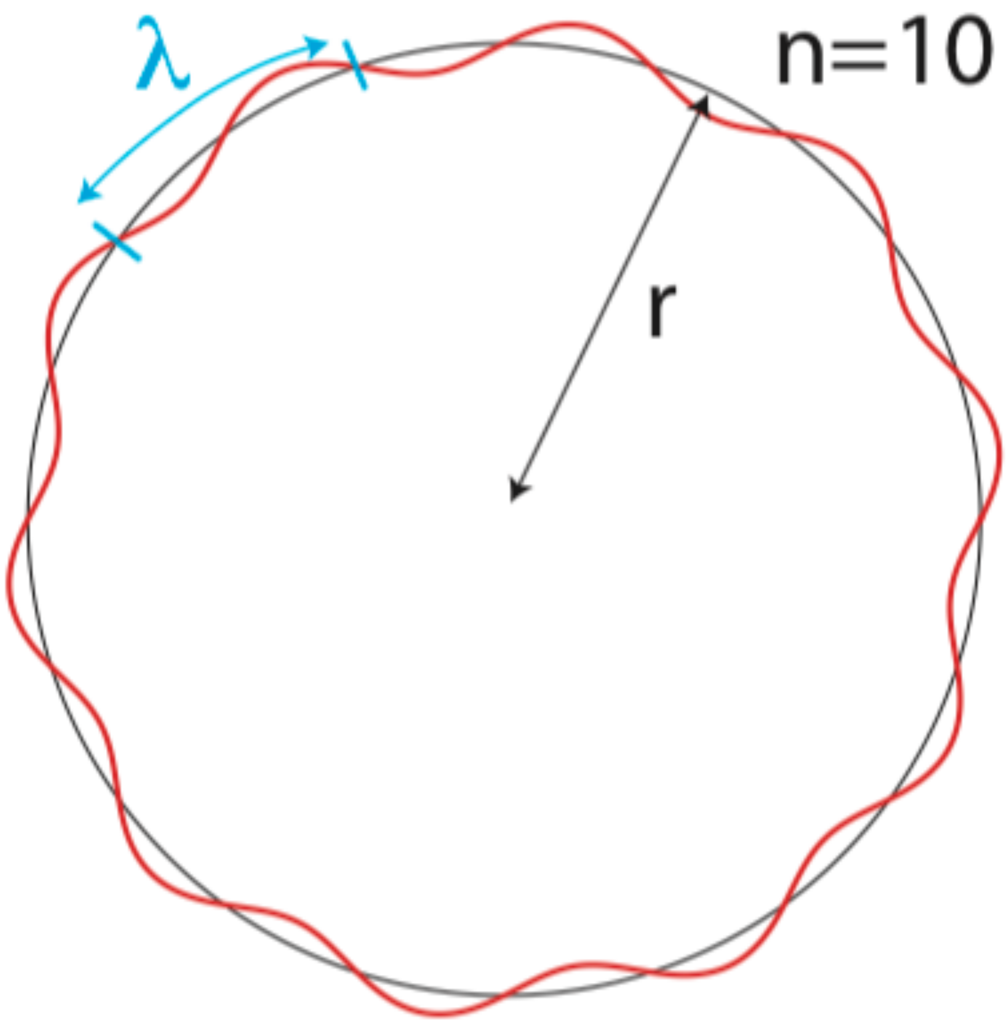
Nobelova za kemijo (1908)

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 → O)
- hipoteza o protonu in nevtronu


THOMSON MODEL
RUTHERFORD MODEL
gold foil
alpha particle source
gold foil
alpha particle source
OBSERVED RESULT

1. 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

$$r_n = n^2 a_0$$

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

Bohrov polmer

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

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

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

1Ry=1Rydberg

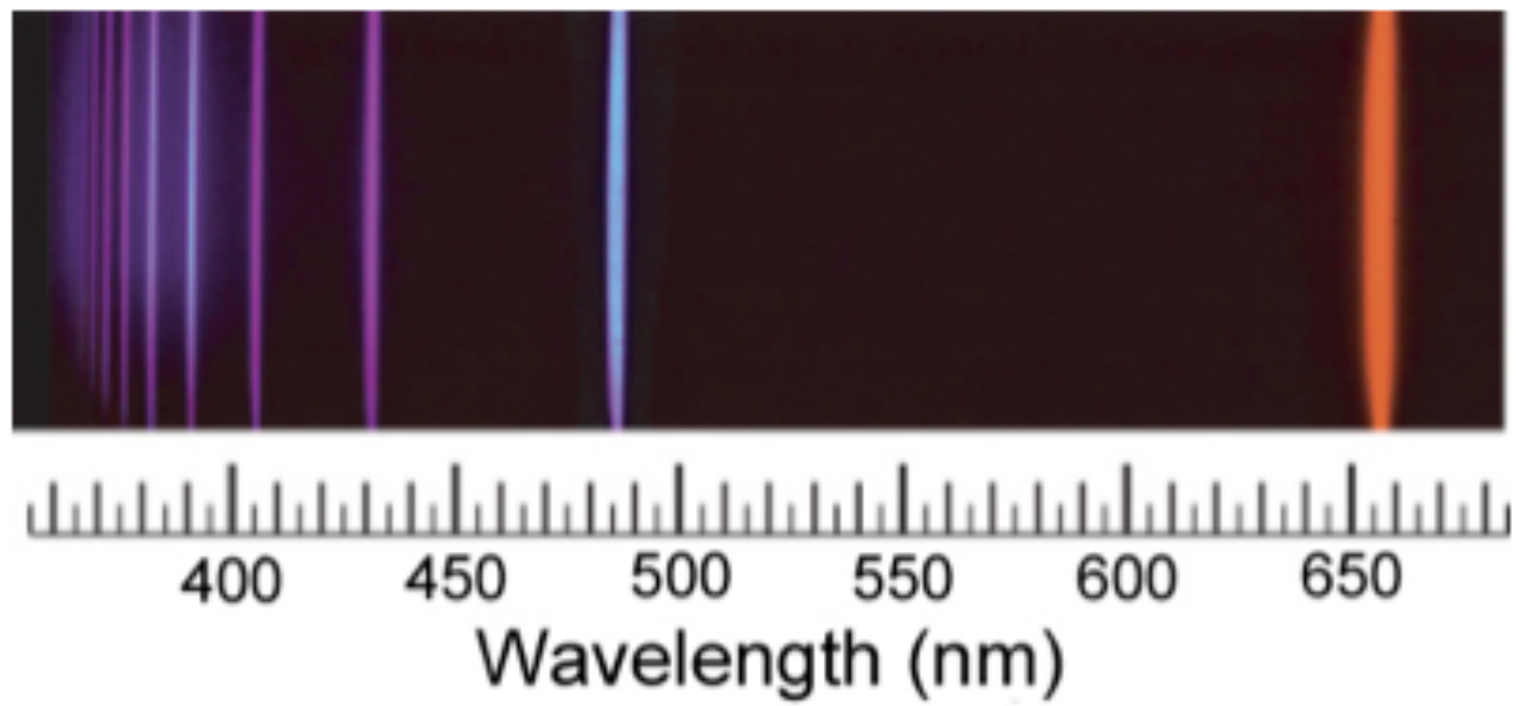
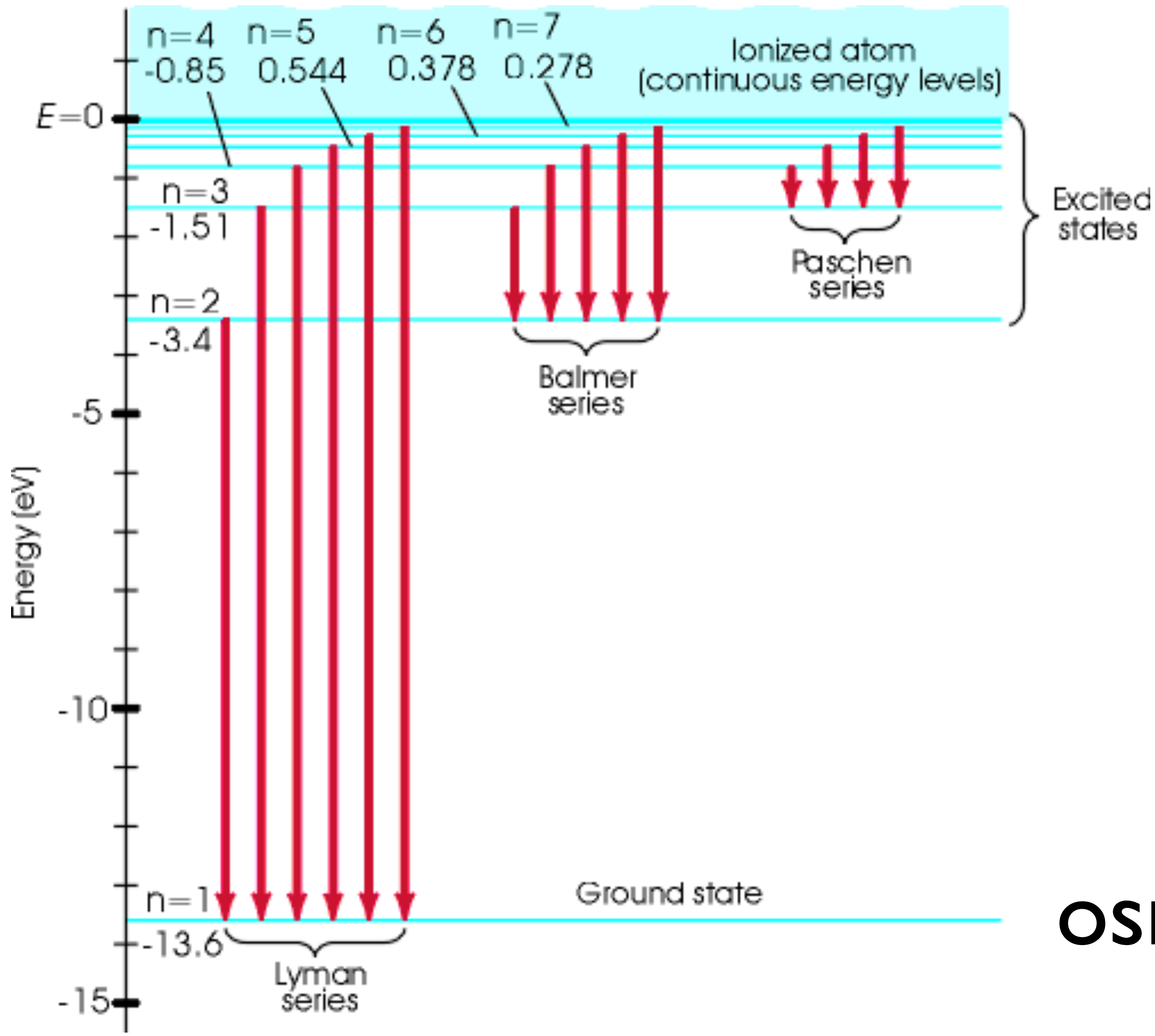
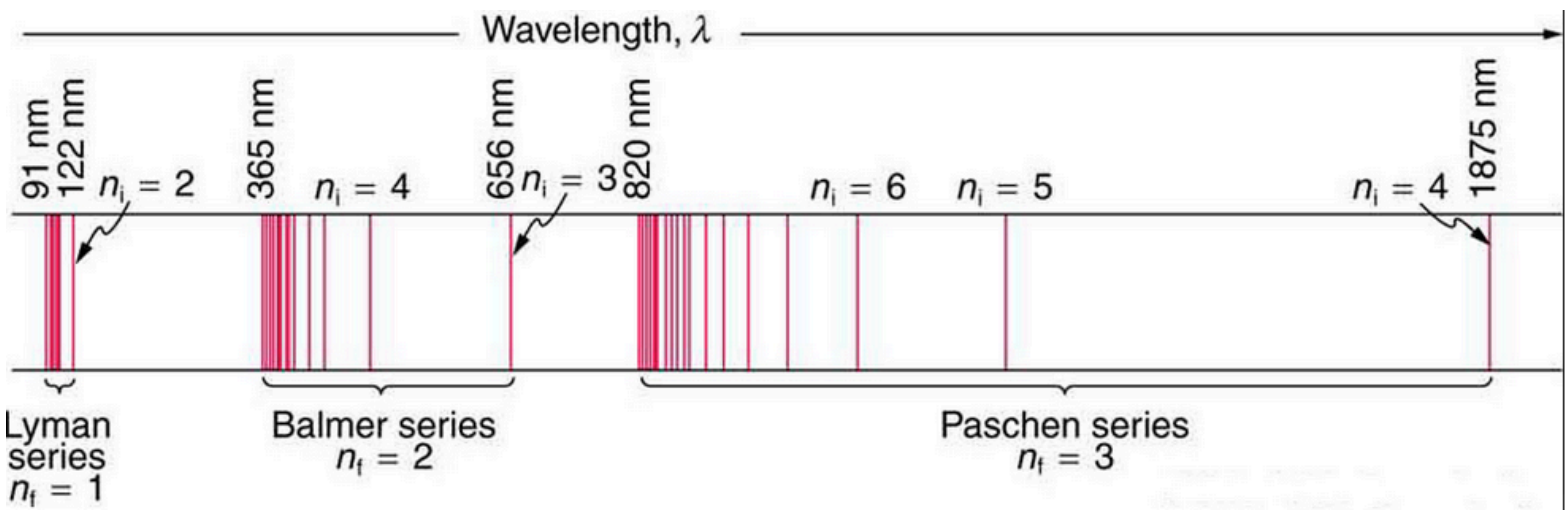


Figure 12: The spectrum of atomic hydrogen.
Source: © T.W. Hänsch.

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



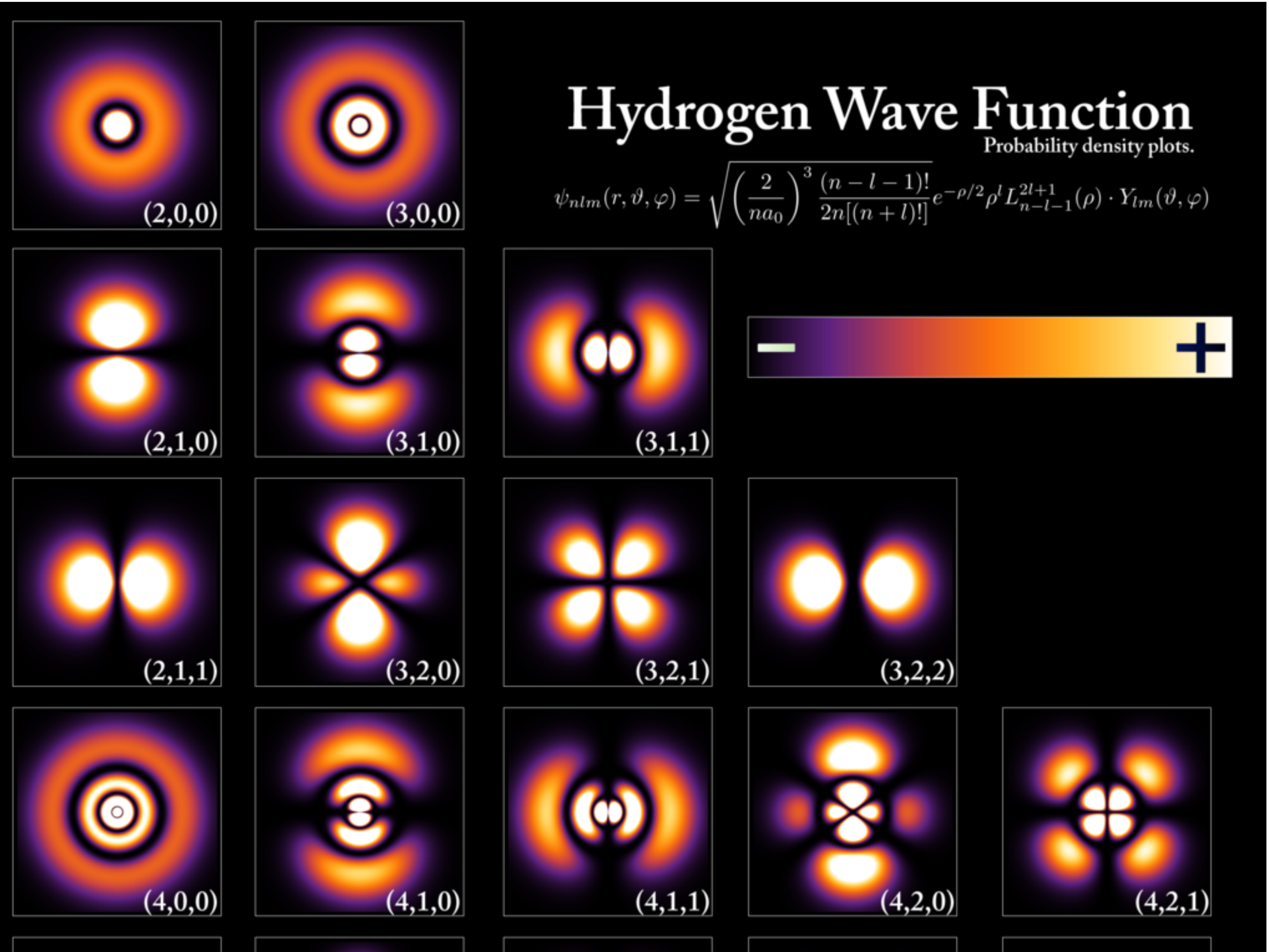
osnovno stanje

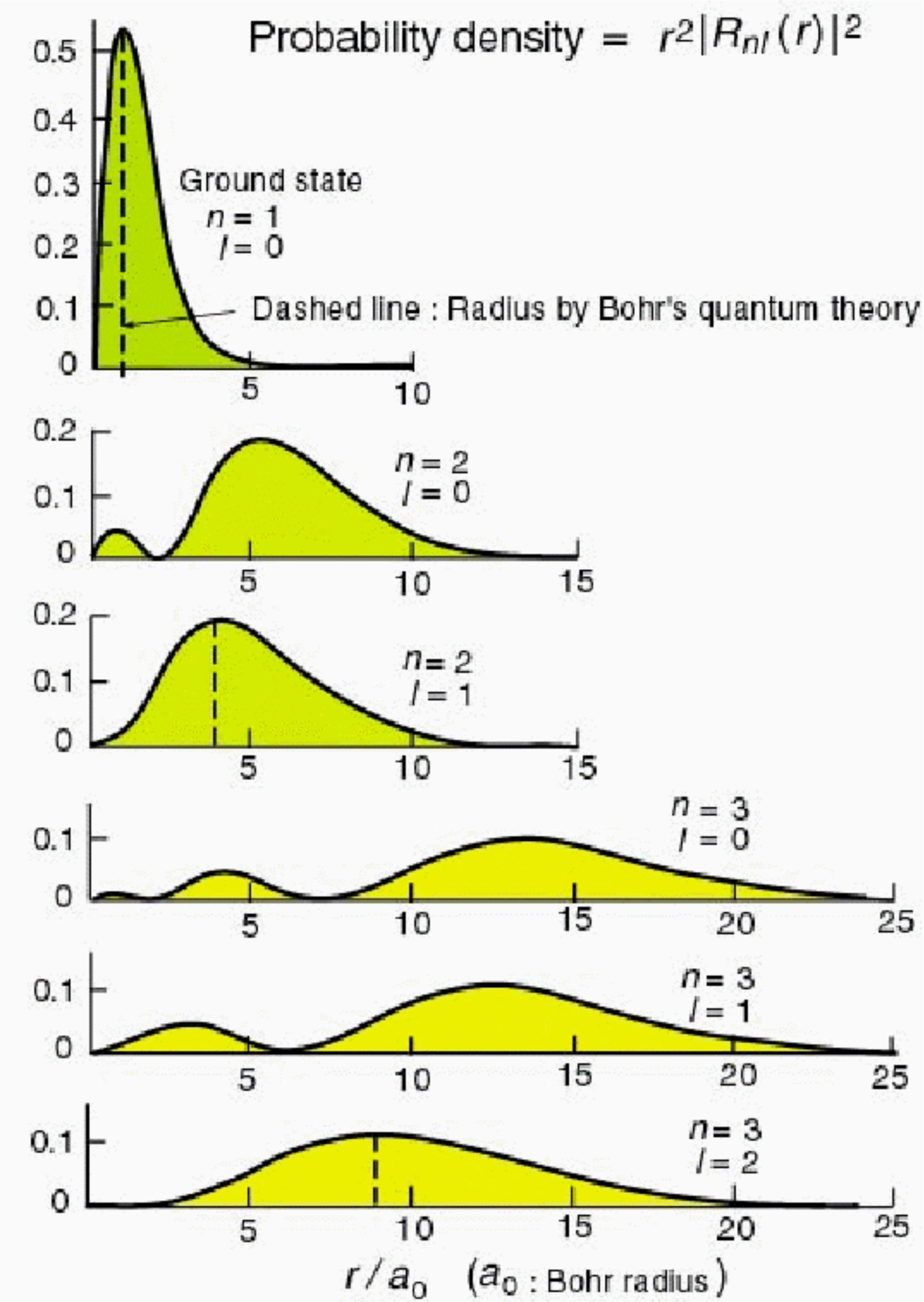


2. Zakaj se lastnosti elementov ponvaljajo periodično?

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

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

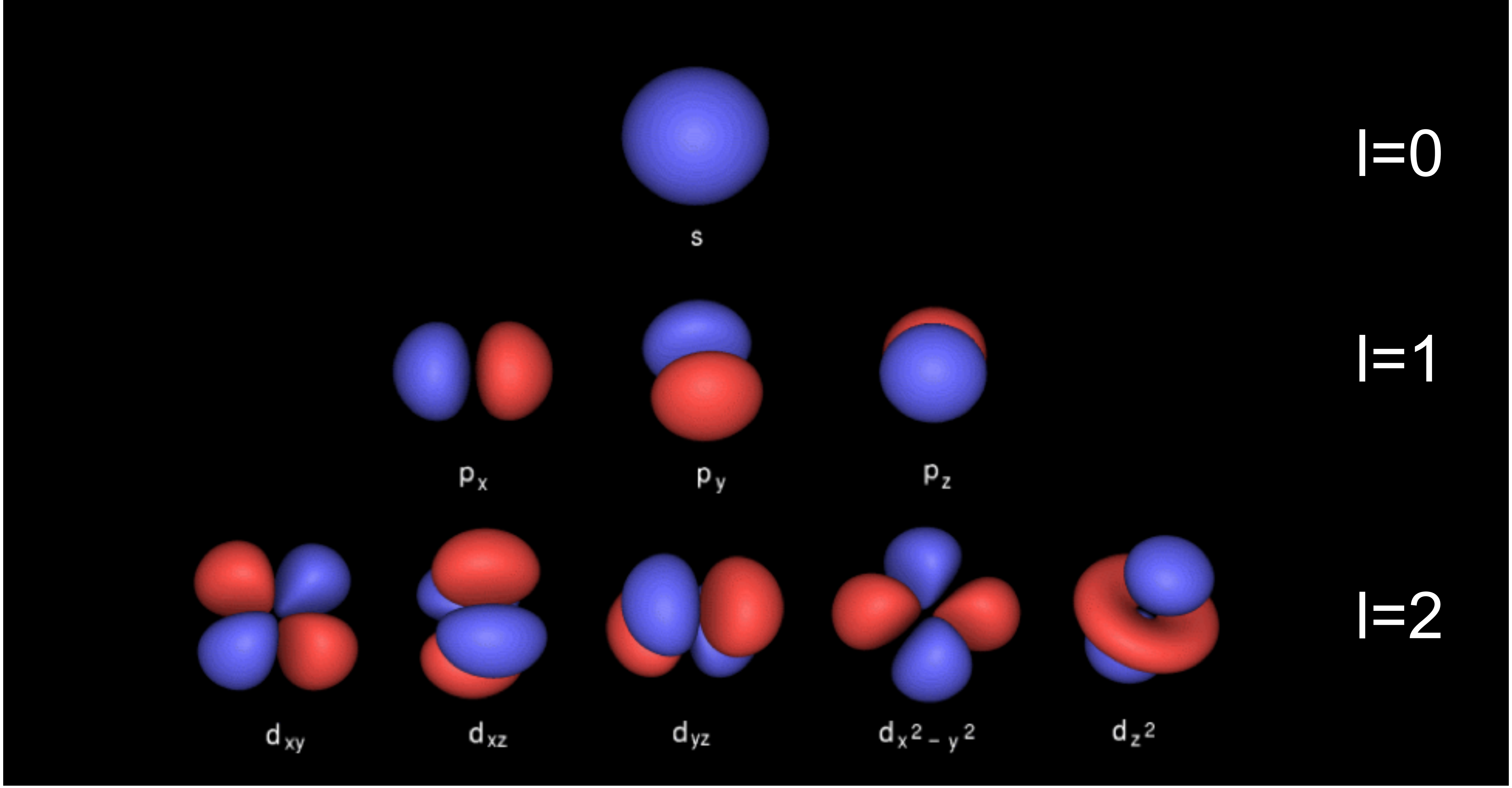

Hydrogen Wave Function
Probability density plots.
$\psi_{nlm}(r,\vartheta,\varphi)=\sqrt{\left(\frac{2}{na_0}\right)^3\frac{(n-l-1)!}{2n[(n+l)!]}}e^{-\rho/2}\rho^l L^{2l+1}_{n-l-1}(\rho)\cdot Y_{lm}(\vartheta,\varphi)$
−
+
(2,0,0)
(3,0,0)
(2,1,0)
(3,1,0)
(3,1,1)
(2,1,1)
(3,2,0)
(3,2,1)
(3,2,2)
(4,0,0)
(4,1,0)
(4,1,1)
(4,2,0)
(4,2,1)



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

n	oznaka
1	K
2	L
3	M
4	N

$$n_r = n - l - 1$$

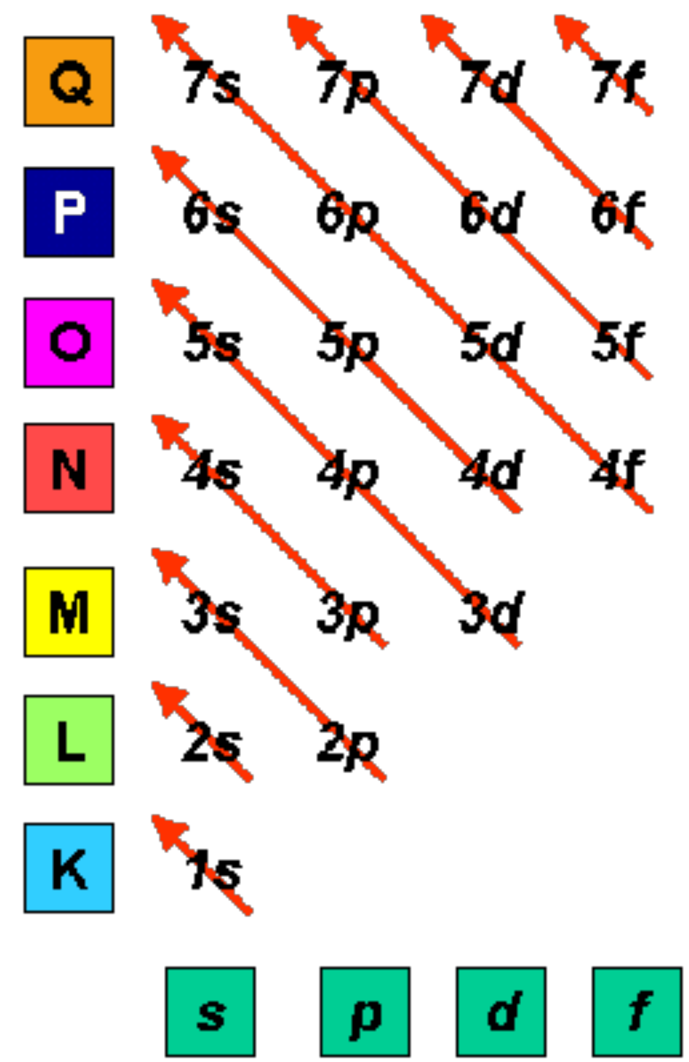


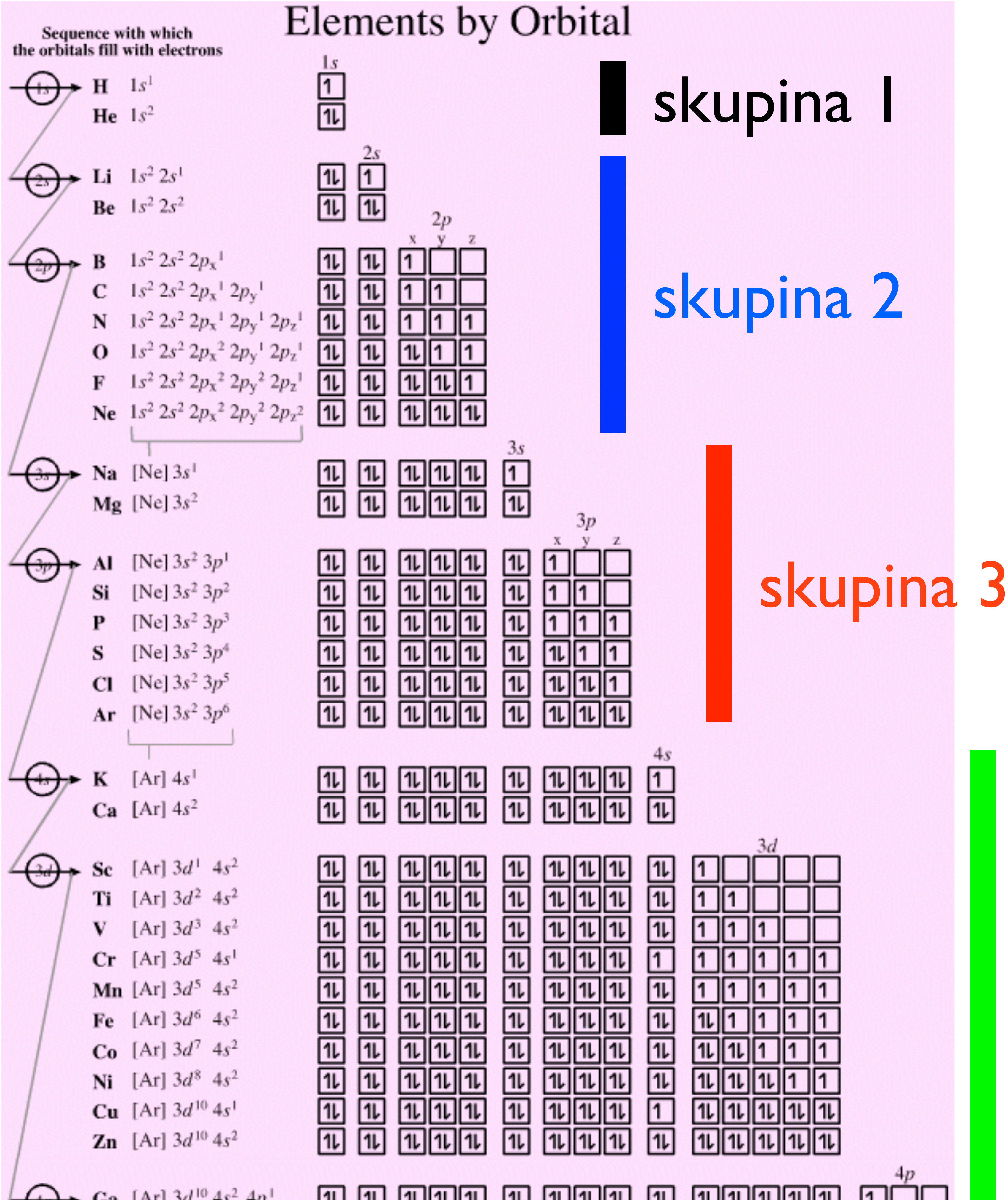
krogelne funkcije (angl. spherical harmonics)

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

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



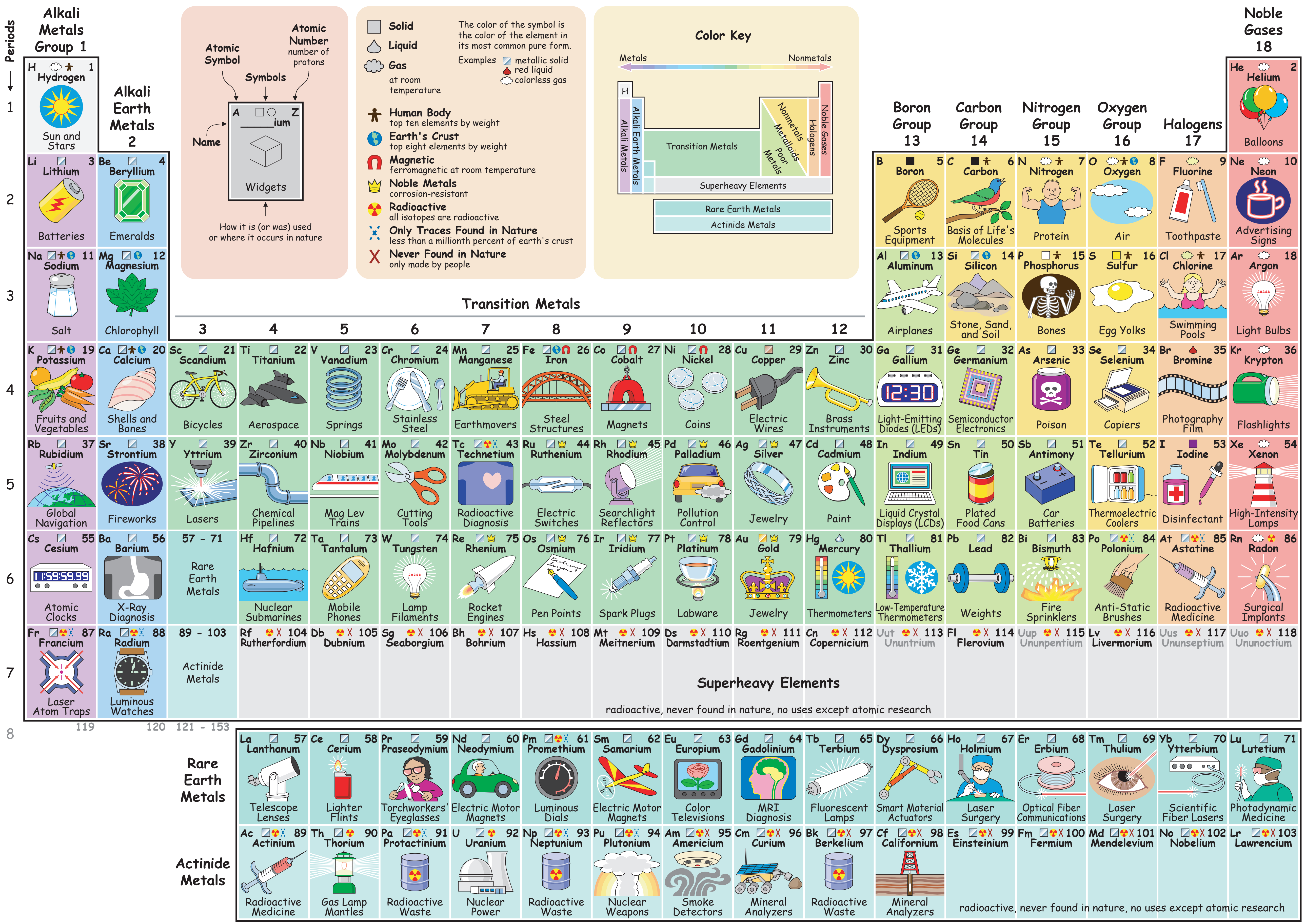


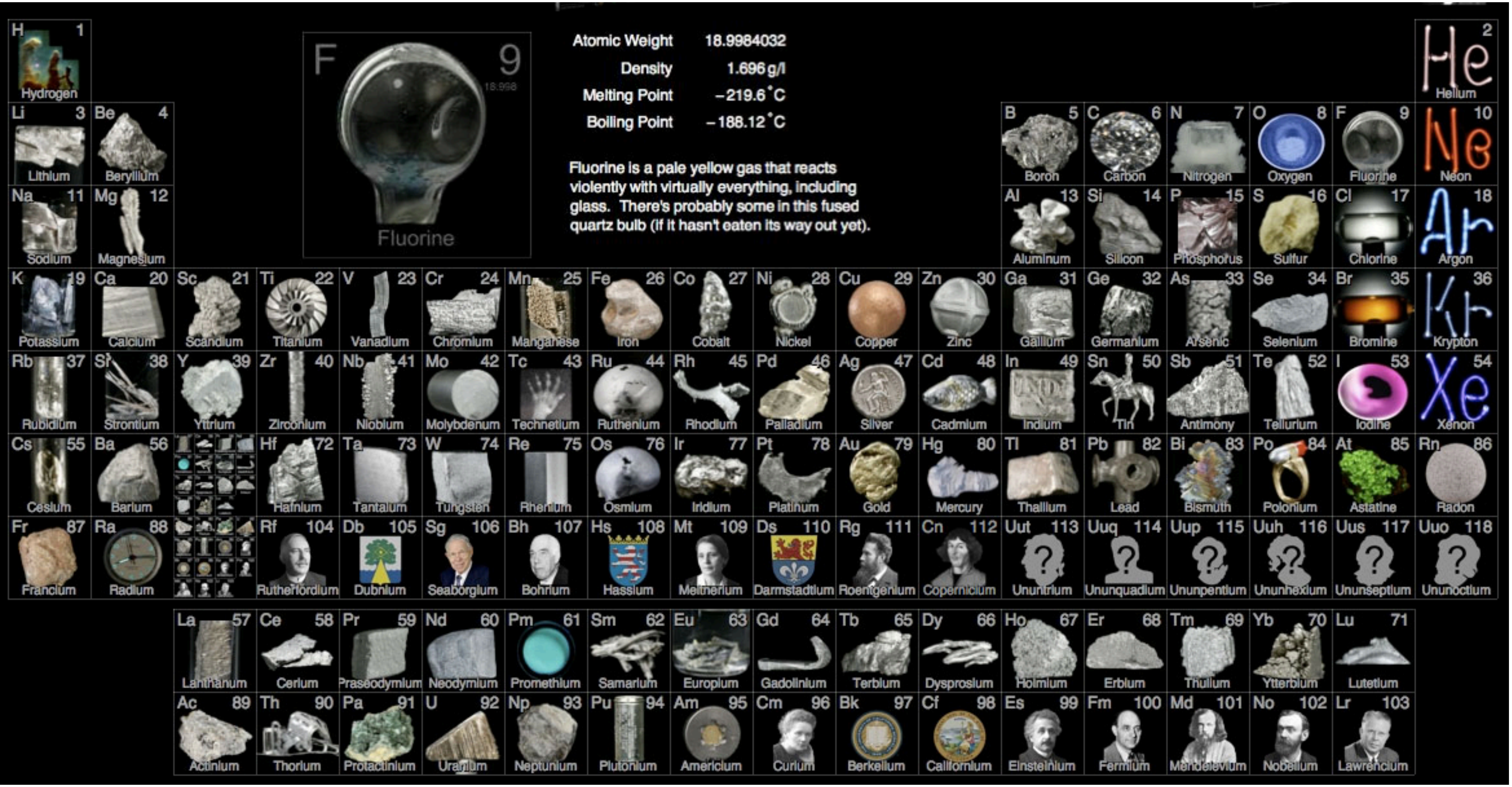
PAULIJEVO IZKLJUČITVENO NAČELO

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

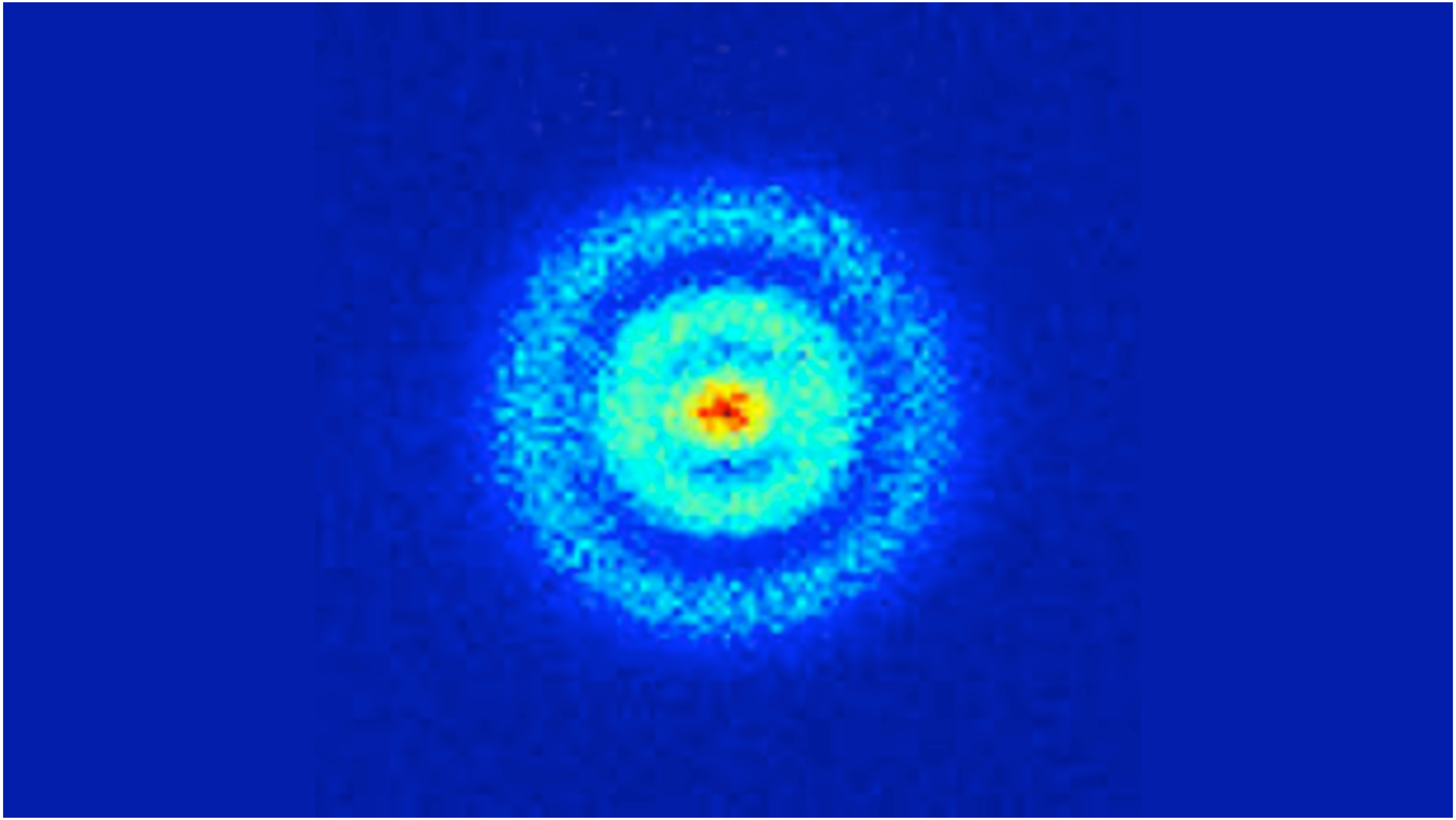




www.periodictable.com

periodic table table

(2002 Ig Nobel Prize in chemistry)



Atom vodika posnet s kvantnim mikroskopom (2013)

Kemijske vezi

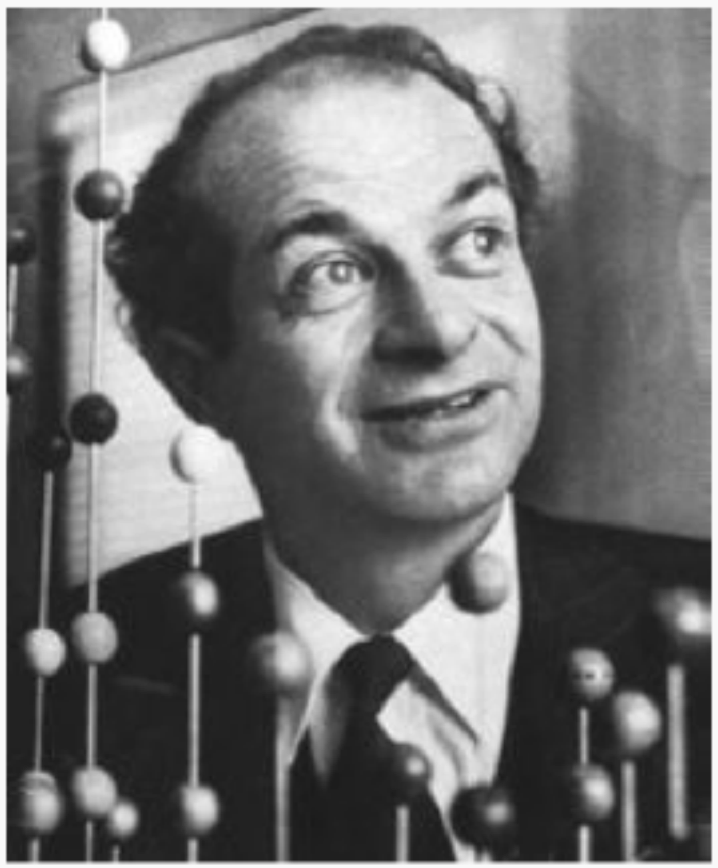
The Parts of all homogeneal hard Bodies which fully touch one another, stick together very strongly. And for explaining how this may be, some have invented hooked Atoms, which is begging the Question; and others tell us that Bodies are glued together by rest, that is, by an occult Quality, or rather 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.

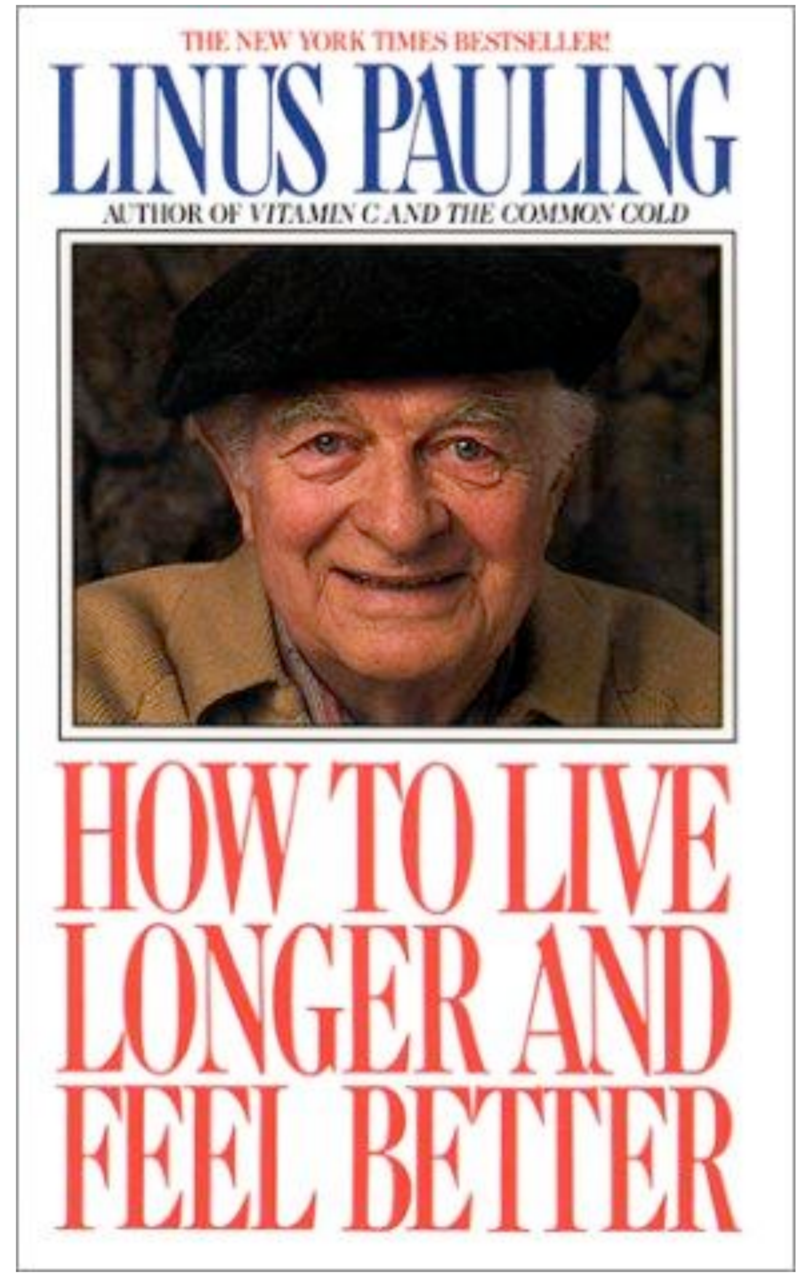
Newton (Opticks, 1704)

kemija

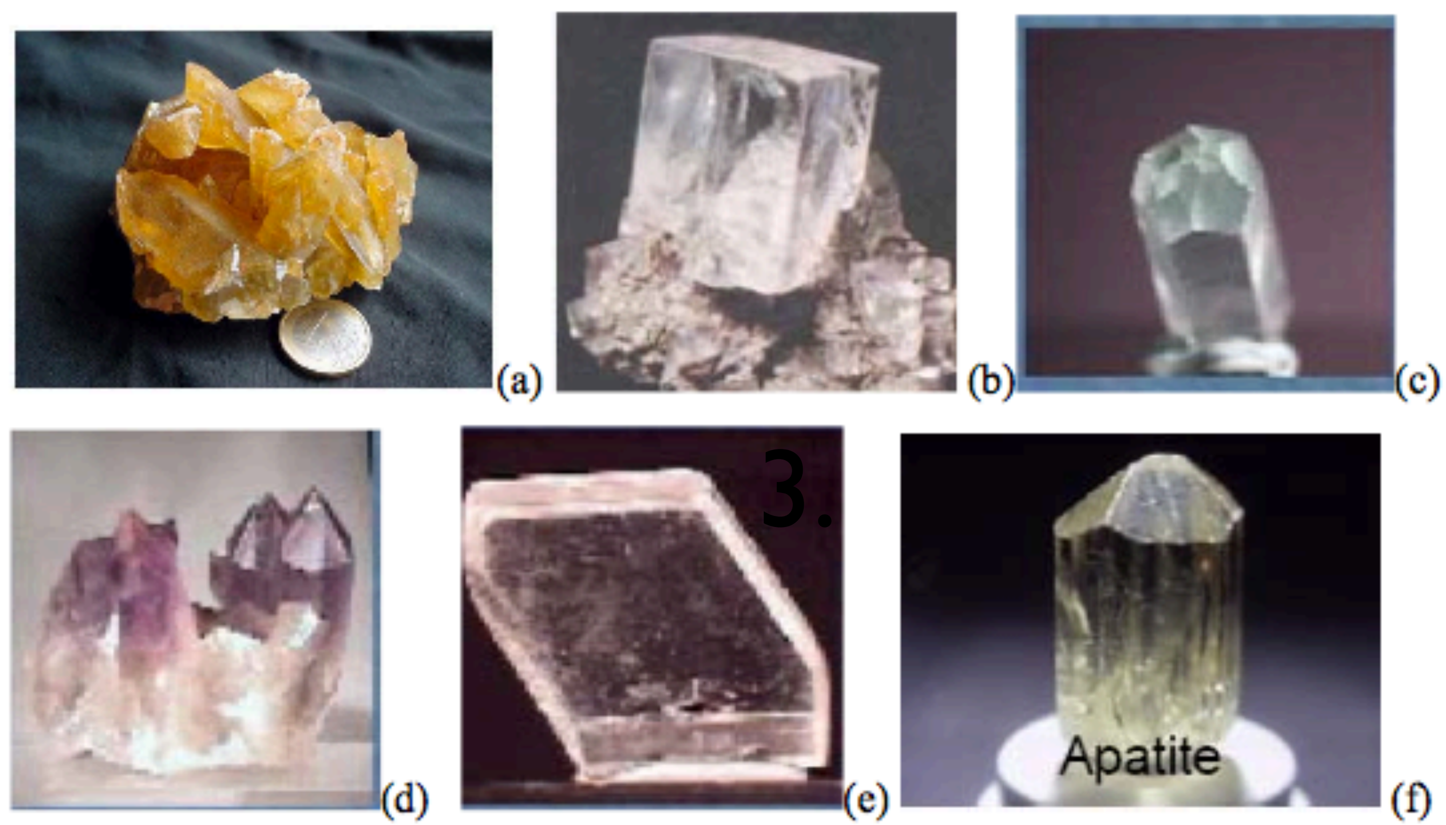
mir

Linus Pauling



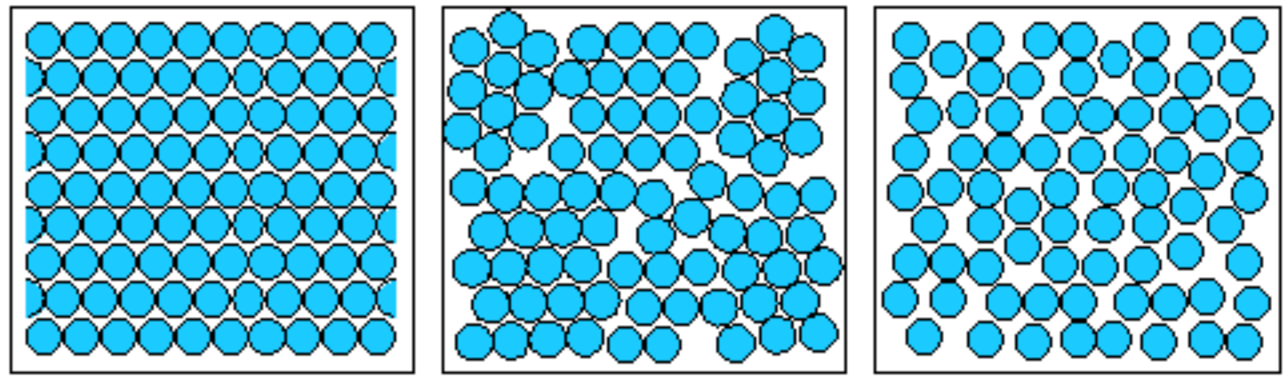


3. Kako opišemo kristalno mrežo?



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

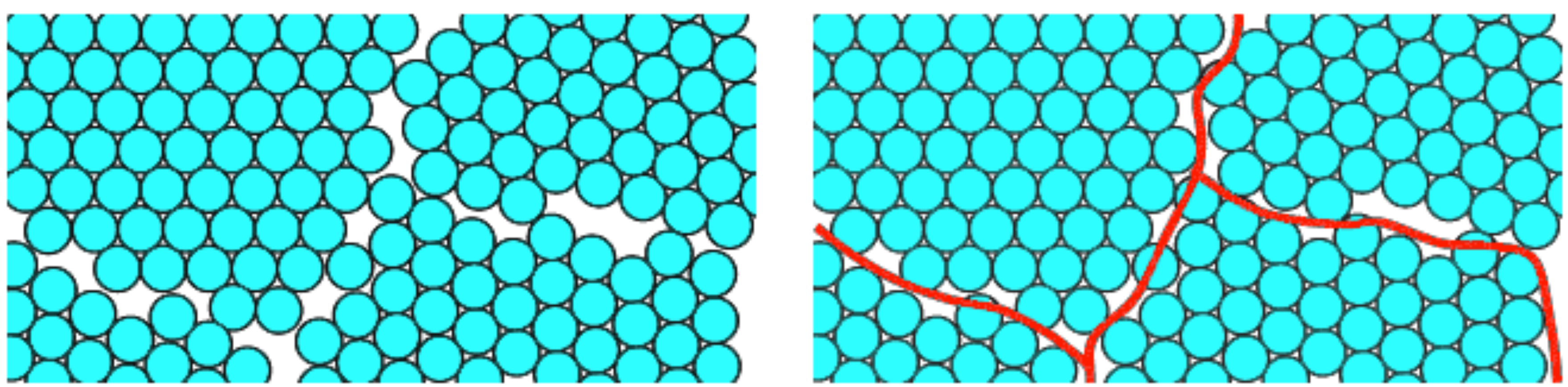
http://webmineral.com/



Single crystal — Periodic across the whole volume.

Polycrystal — Periodic across each grain.

Amorphous solid — Not periodic.

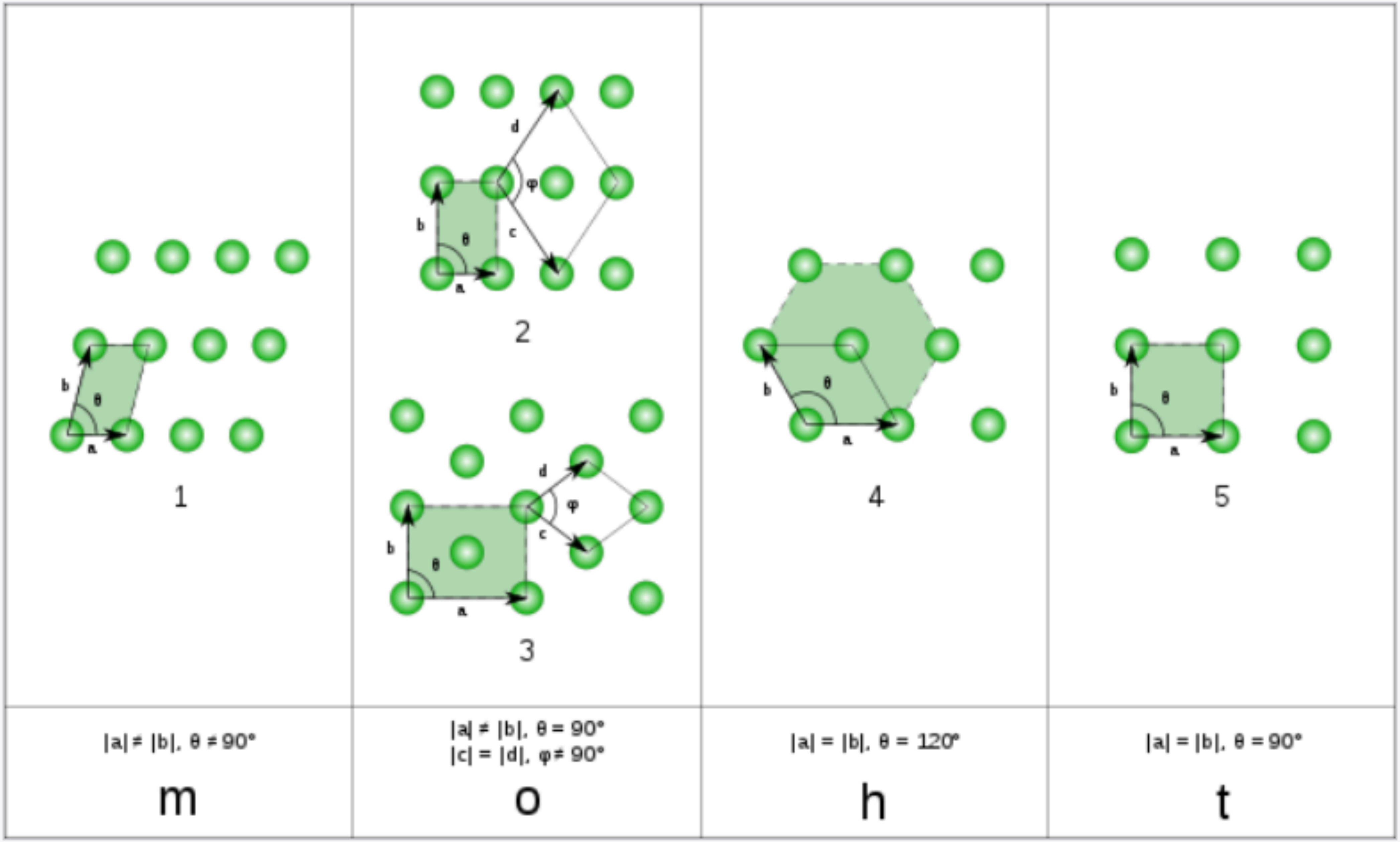


Slika 9.5. Kristalna mreža = Bravaisova mreža + baza (atomi v osnovni celici).

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

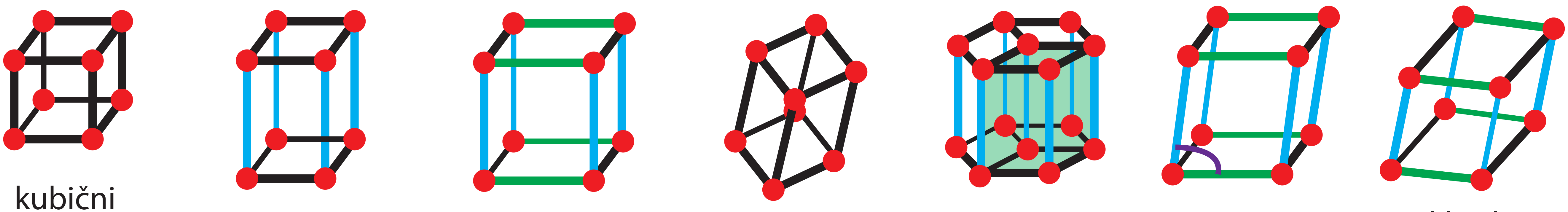
$$\mathbf{r}_j = x_j\mathbf{a}_1 + y_j\mathbf{a}_2 + z_j\mathbf{a}_3$$

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



1 – oblique (monoclinic), 2 – rectangular (orthorhombic), 3 – centered rectangular (orthorhombic), 4 – hexagonal, and 5 – square (tetragonal).

7 sistemov:



kubični
a=b=c
$\alpha=\beta=\gamma=90°$

tetragonalni
a=b≠c
$\alpha=\beta=\gamma=90°$

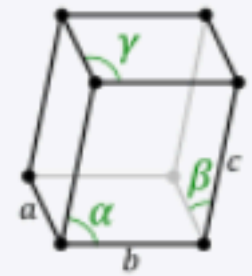
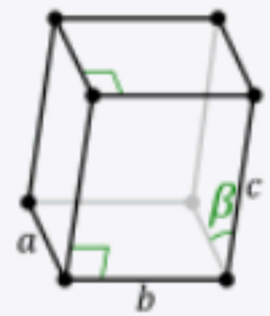
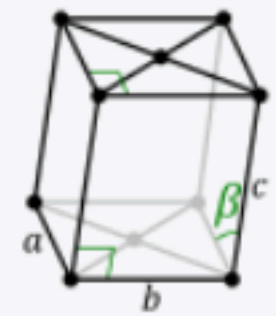
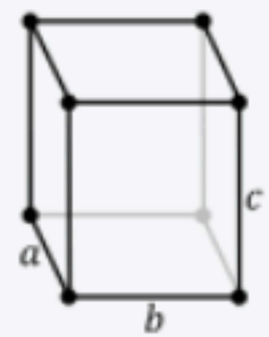
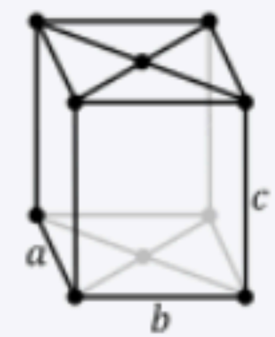
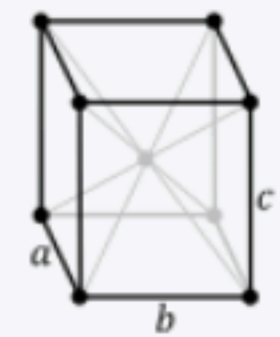
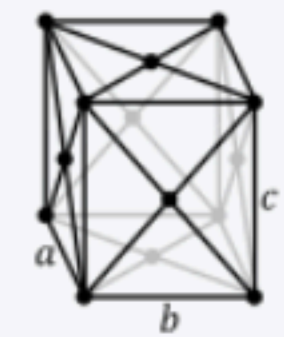
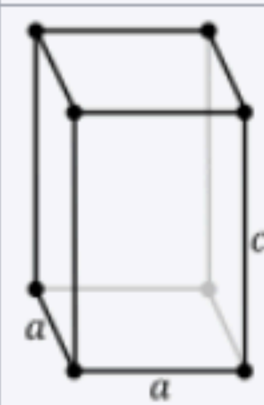
ortorombski
a≠b≠c
$\alpha=\beta=\gamma=90°$

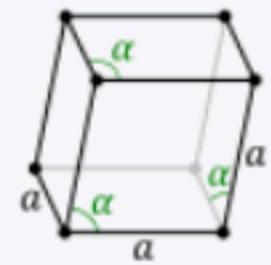
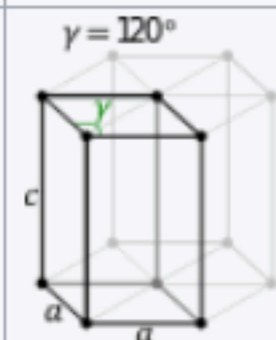
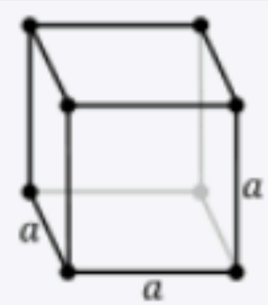
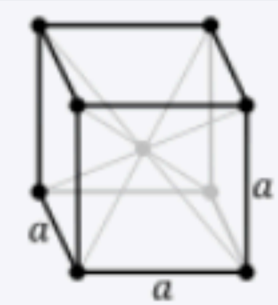
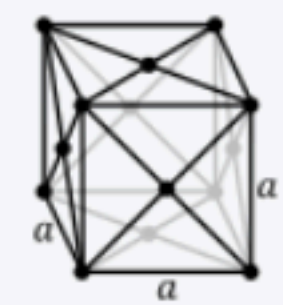
romboedrični
a=b=c
$\alpha=\beta=\gamma\neq 90°$

heksagonalni
a=b≠c
$\alpha=\gamma=90°$
$\beta=120°$

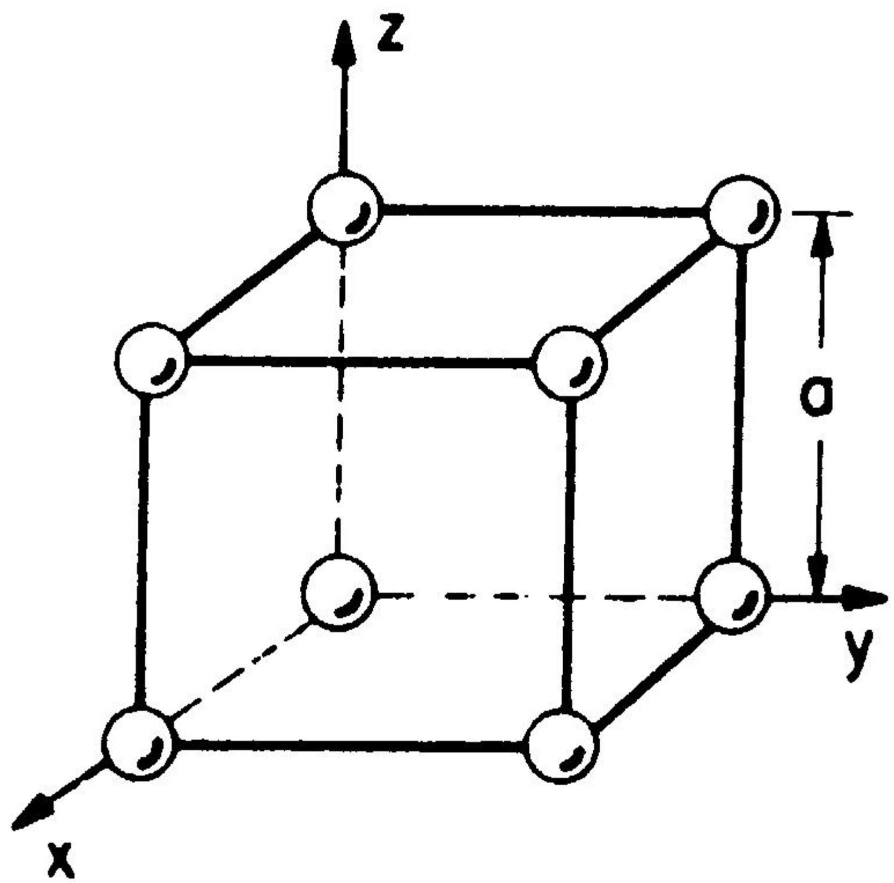
monoklinski
a≠b≠c
$\alpha=\gamma=90°\neq\beta$

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

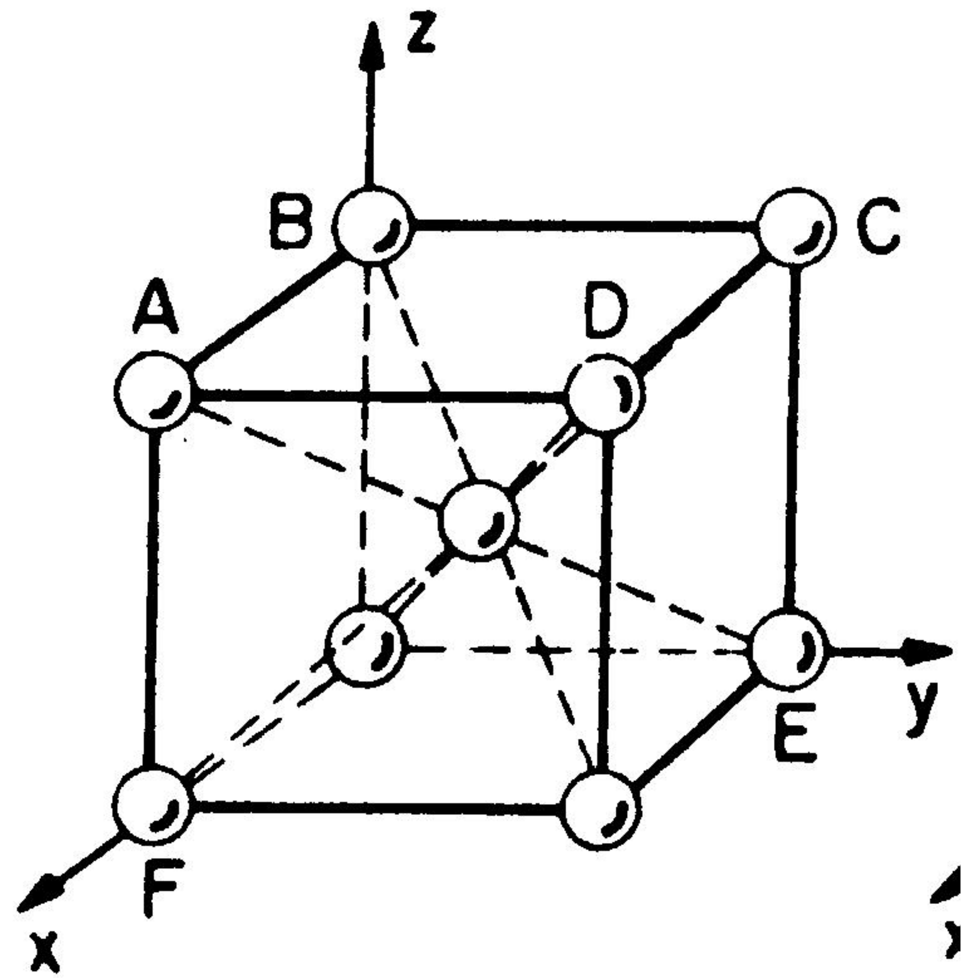
Crystal family	Lattice system	Schönflies	14 Bravais lattices			
			Primitive (P)	Base-centered (C)	Body-centered (I)	Face-centered (F)
Triclinic		C_i				
Monoclinic		C_{2h}				
Orthorhombic		D_{2h}				
Tetragonal		D_{4h}				

Hexagonal	**Rhombohedral**	D_{3d}				
	Hexagonal	D_{6h}				
Cubic		O_h				

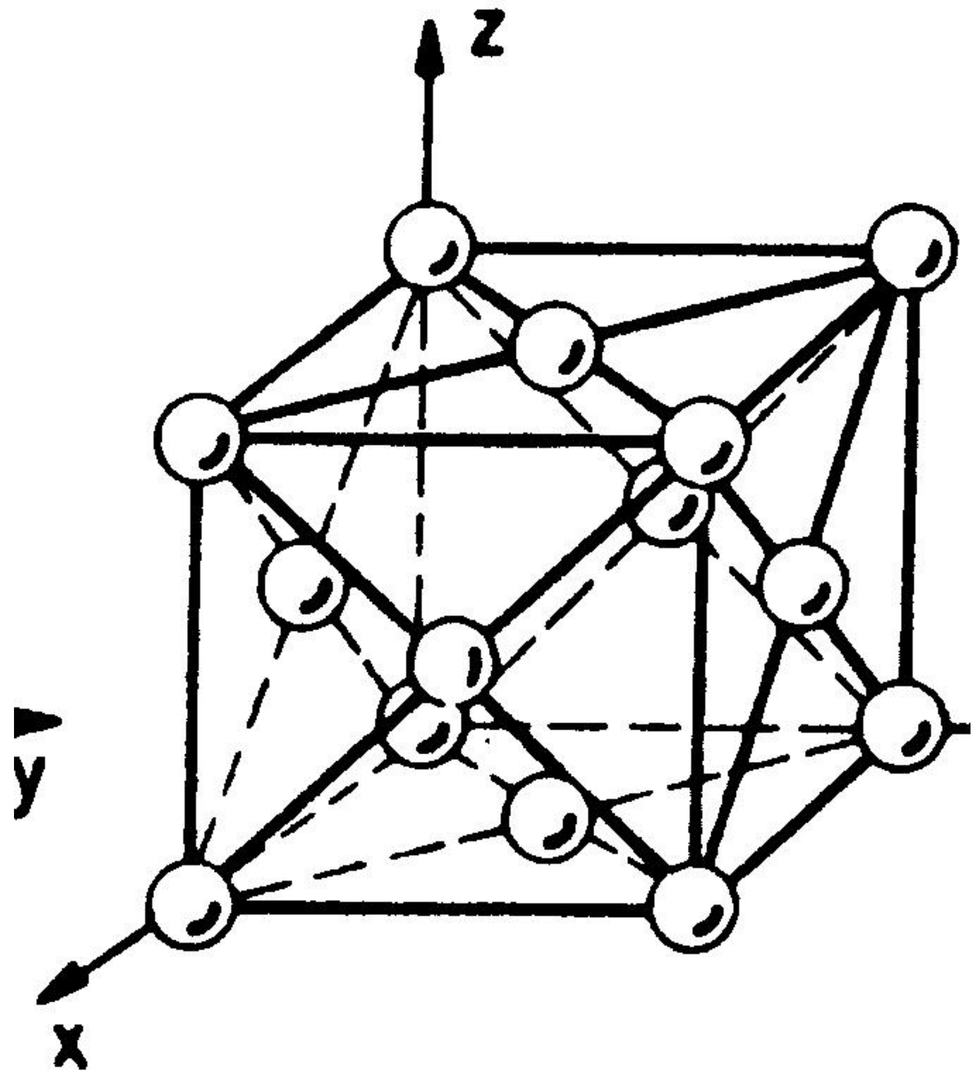
kubični



telesno centriran kubični

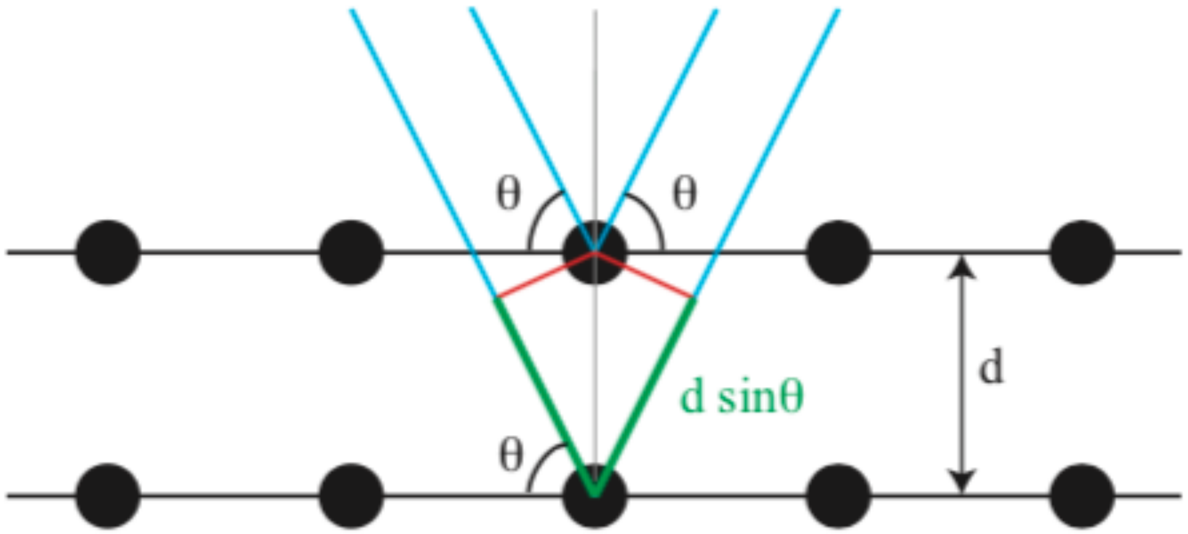


ploskovno centriran kubični



4. Kako določamo kristalno strukturo?

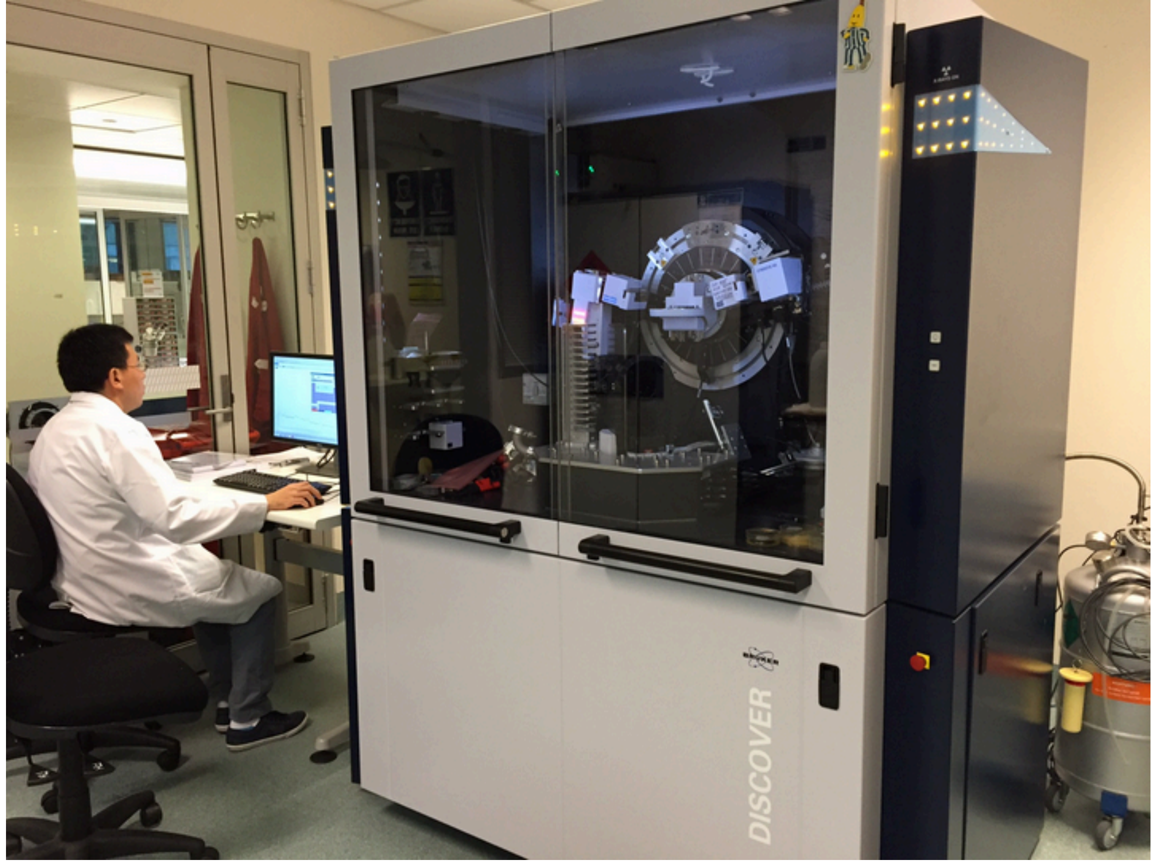
uklon rentgenski žarkov

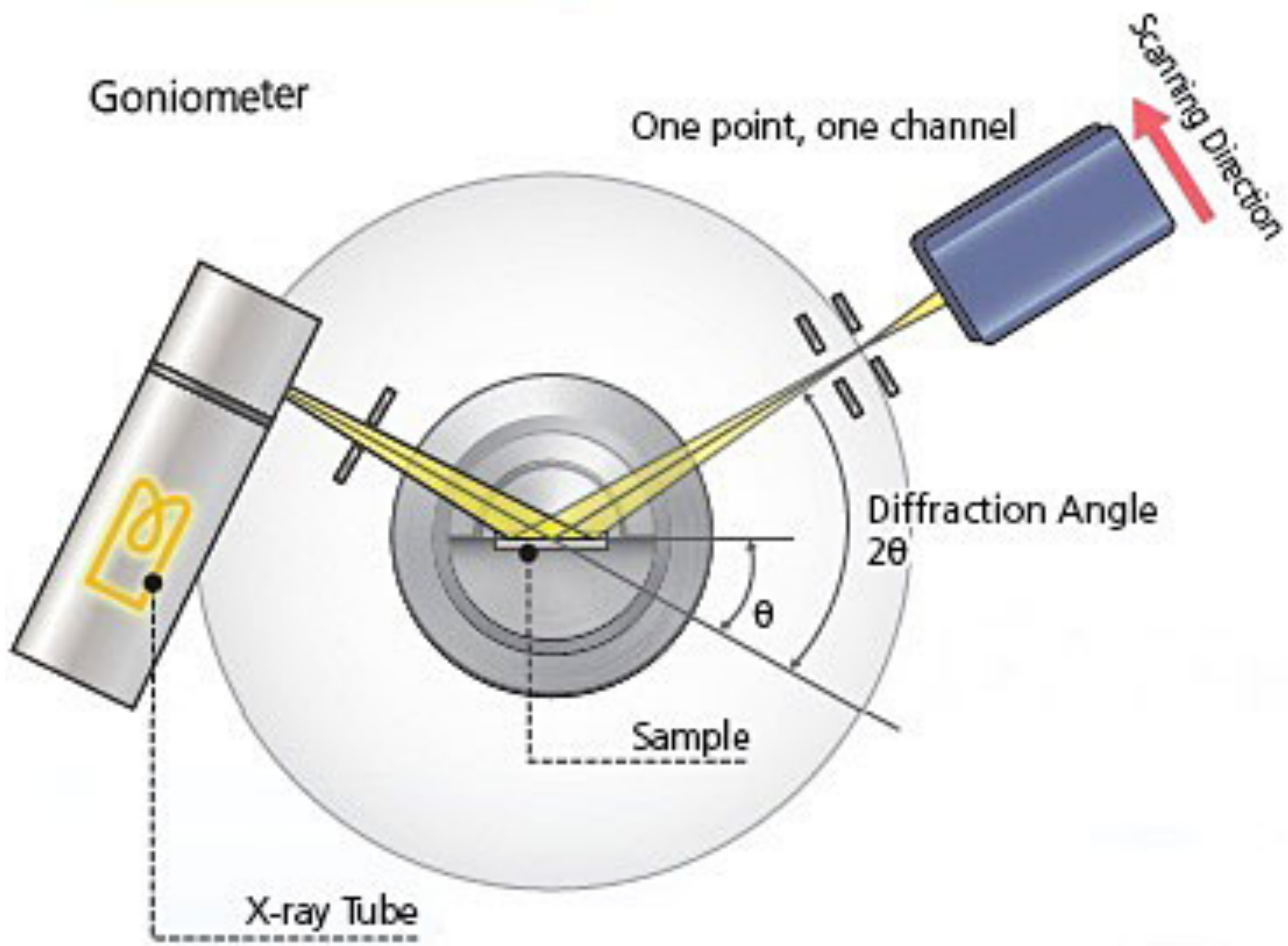


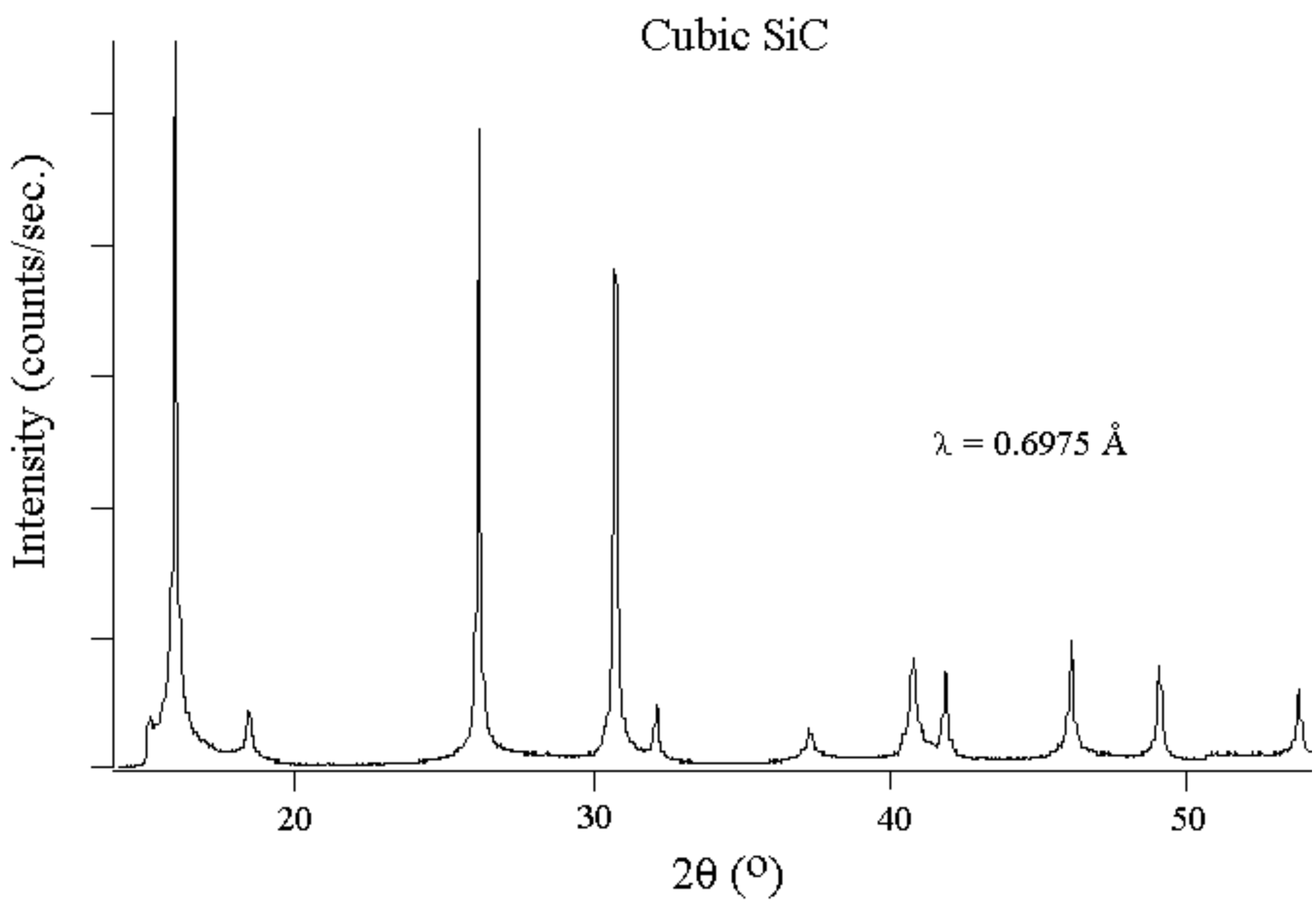
$$n\lambda = 2d\sin\theta$$

Bragg, Laue, ~1912

θ sipalni kot

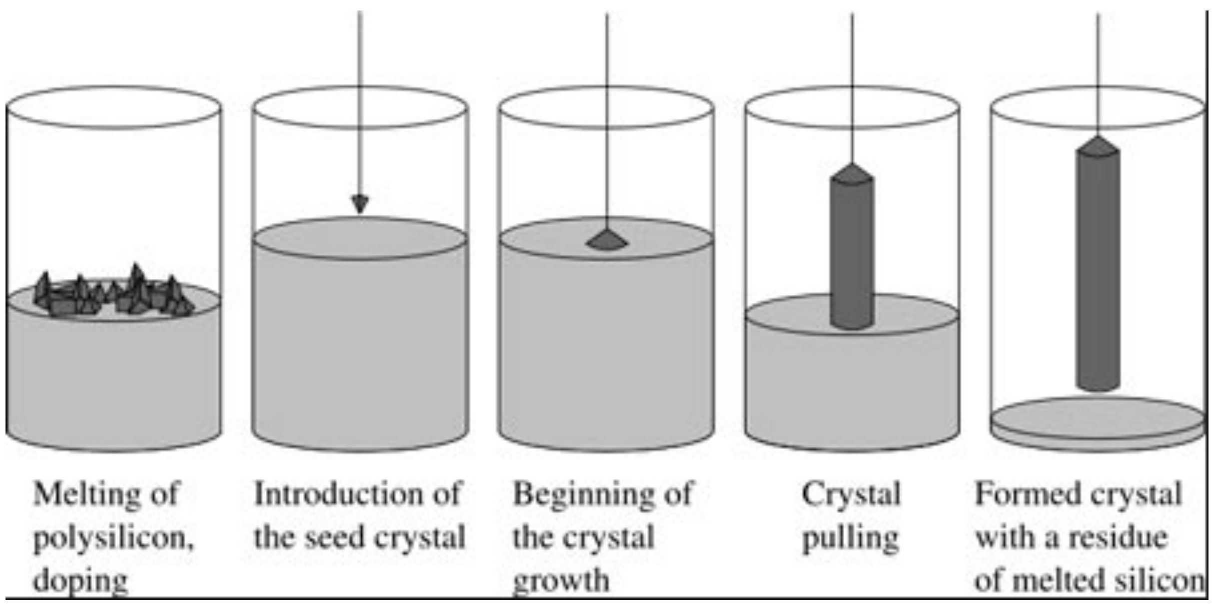

DISCOVER

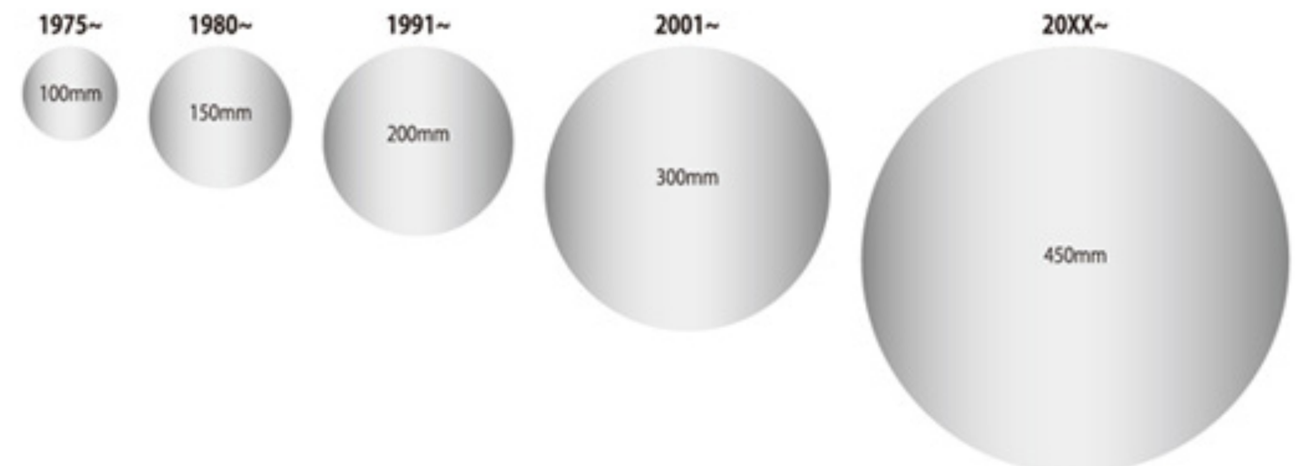

Goniometer
One point, one channel
Scanning Direction
Diffraction Angle
2θ
θ
Sample
X-ray Tube



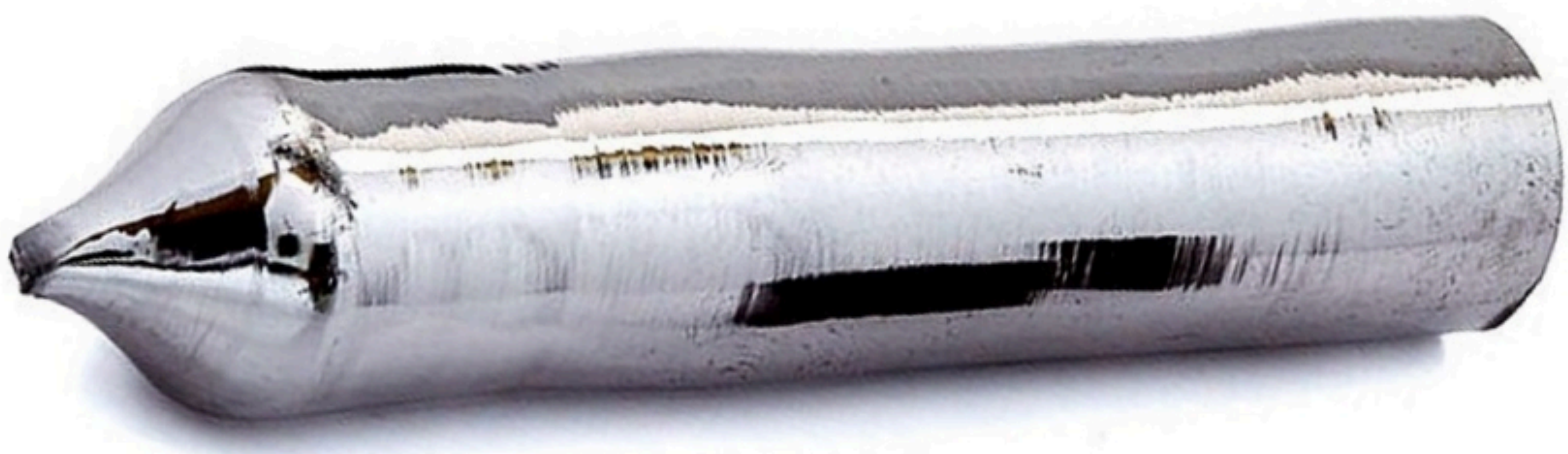
Cubic SiC
Intensity (counts/sec.)
λ = 0.6975 Å
20
30
40
50
2θ (o)

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

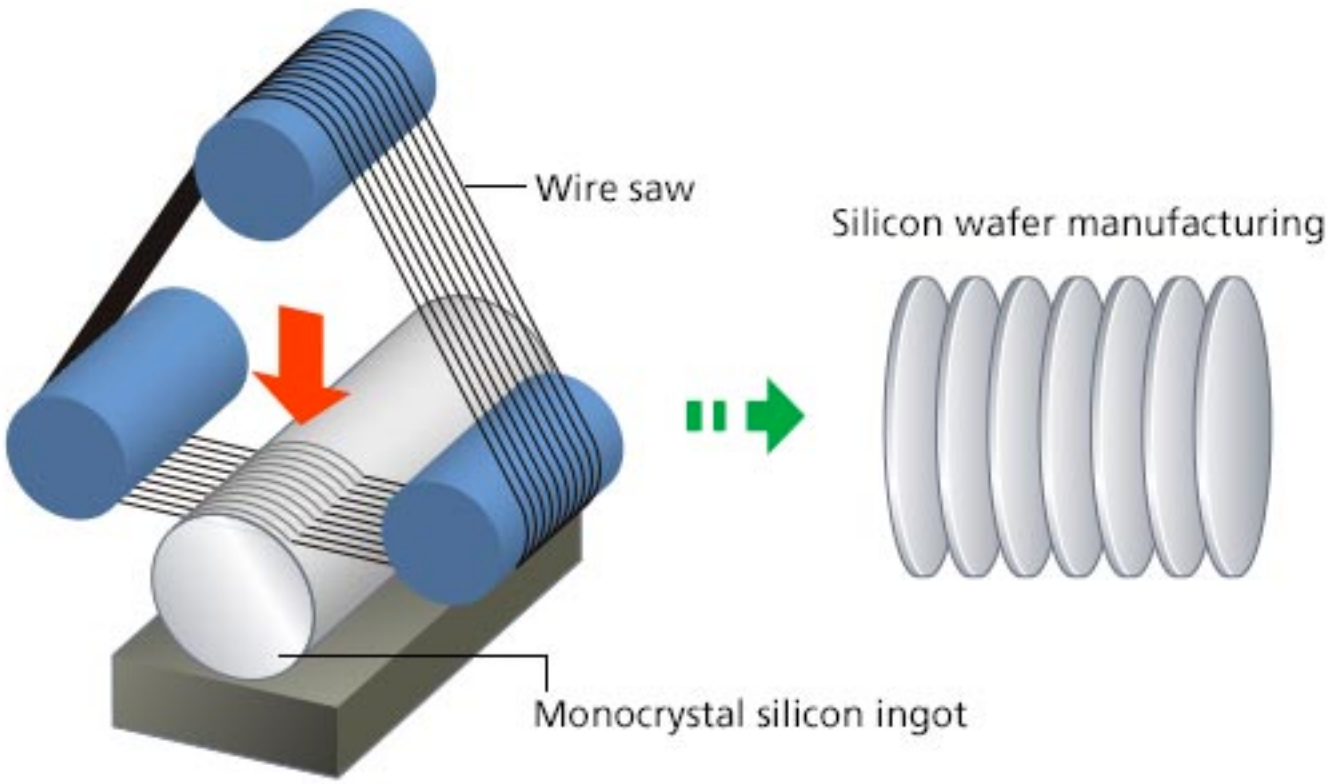




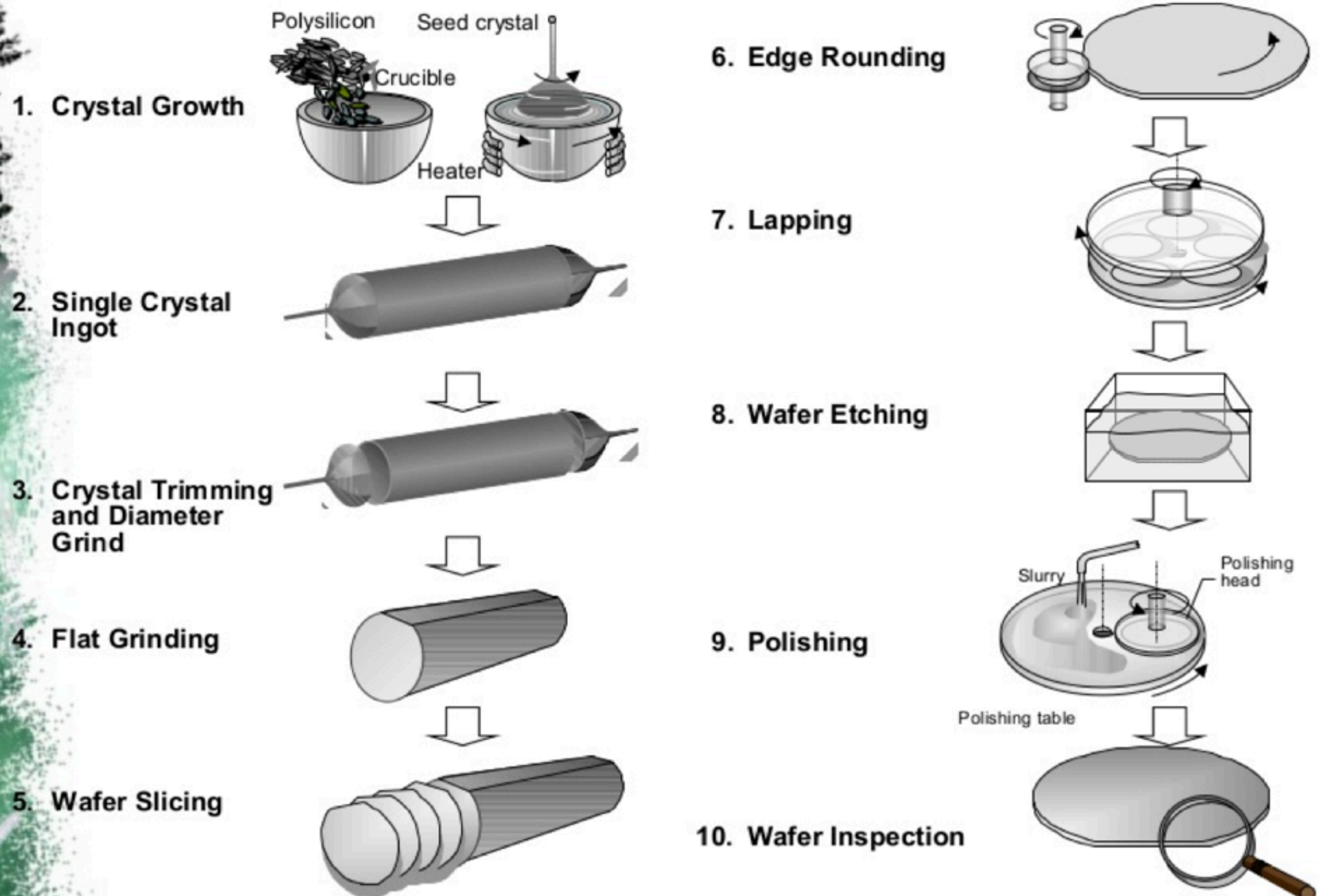
Czochralski




4
5

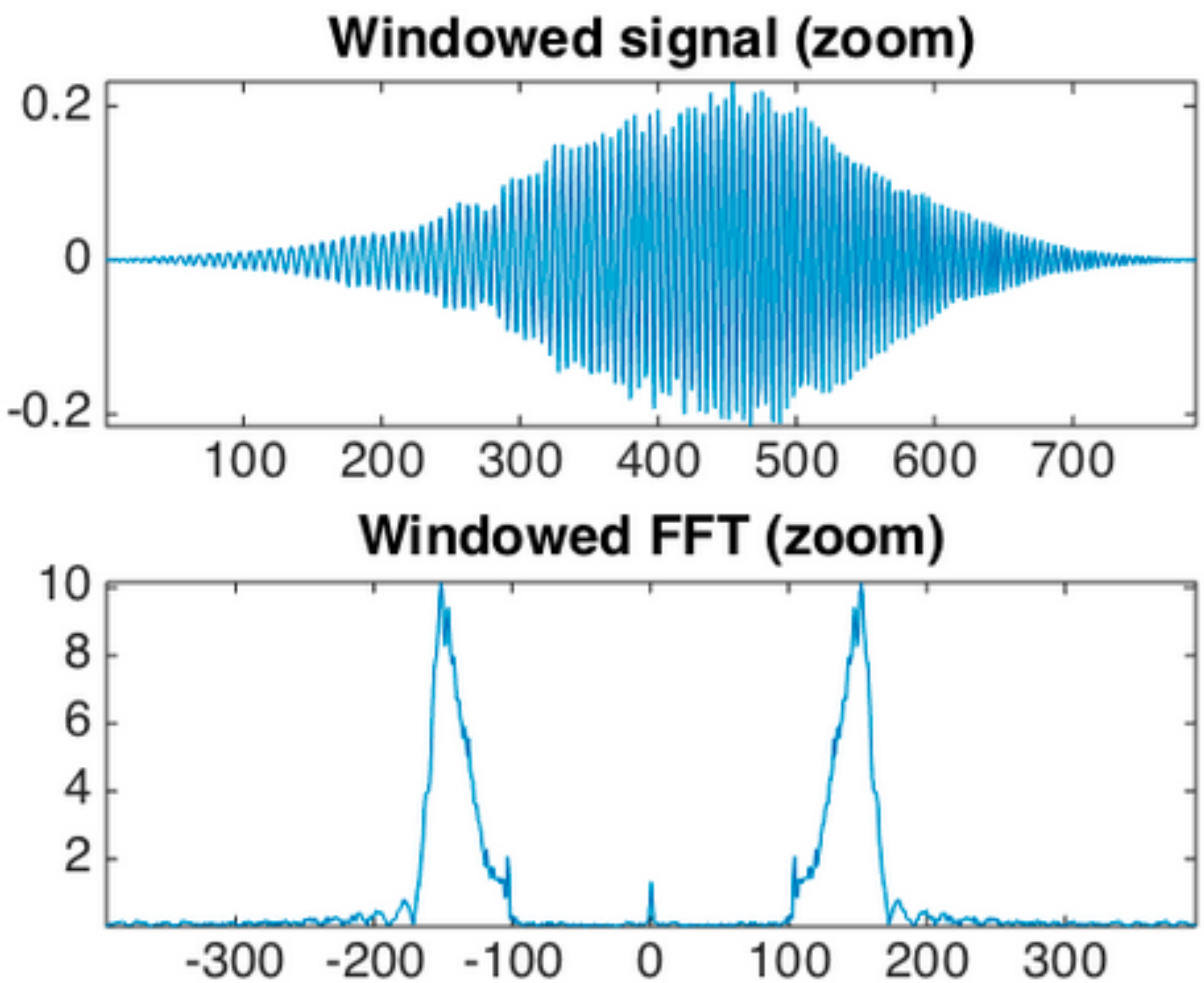

Wire saw
Silicon wafer manufacturing
Monocrystal silicon ingot

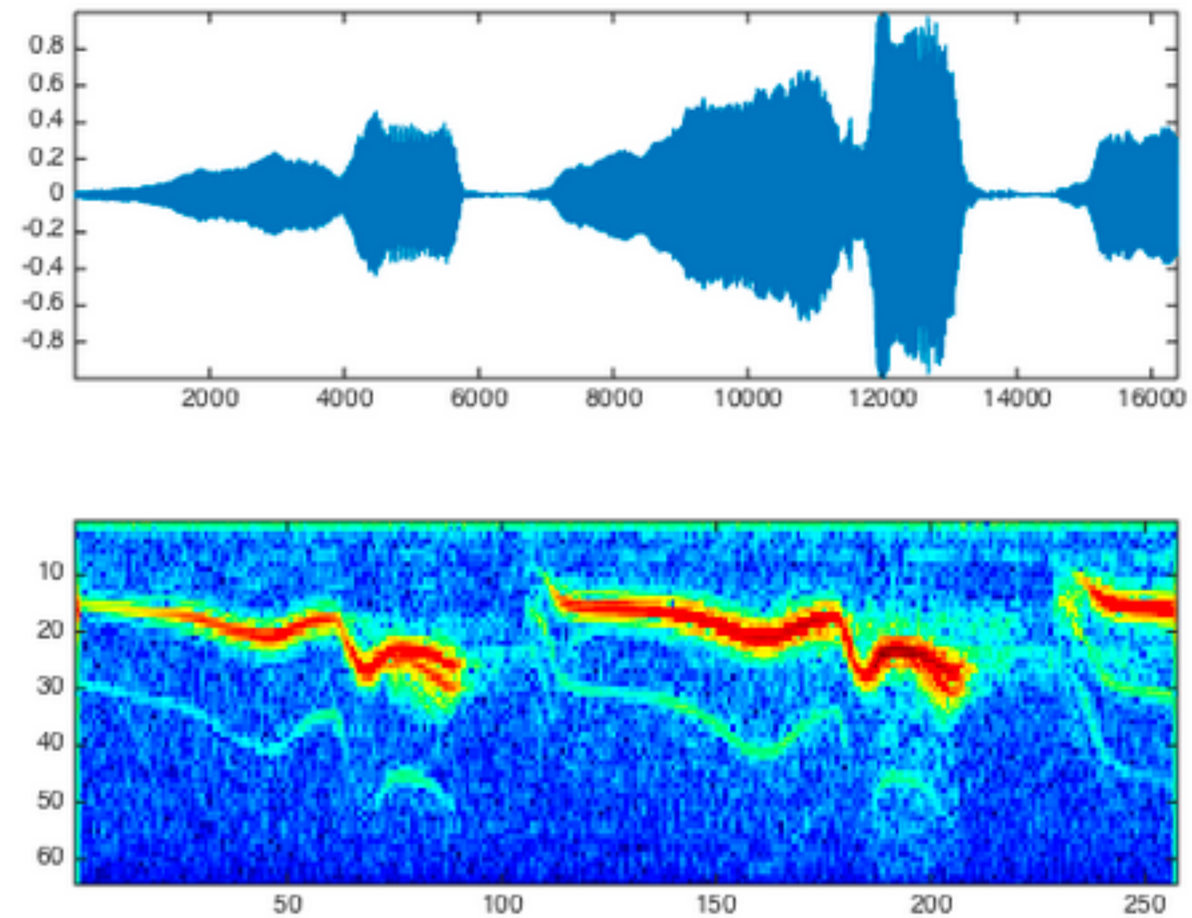
Preparation of Silicon Wafer



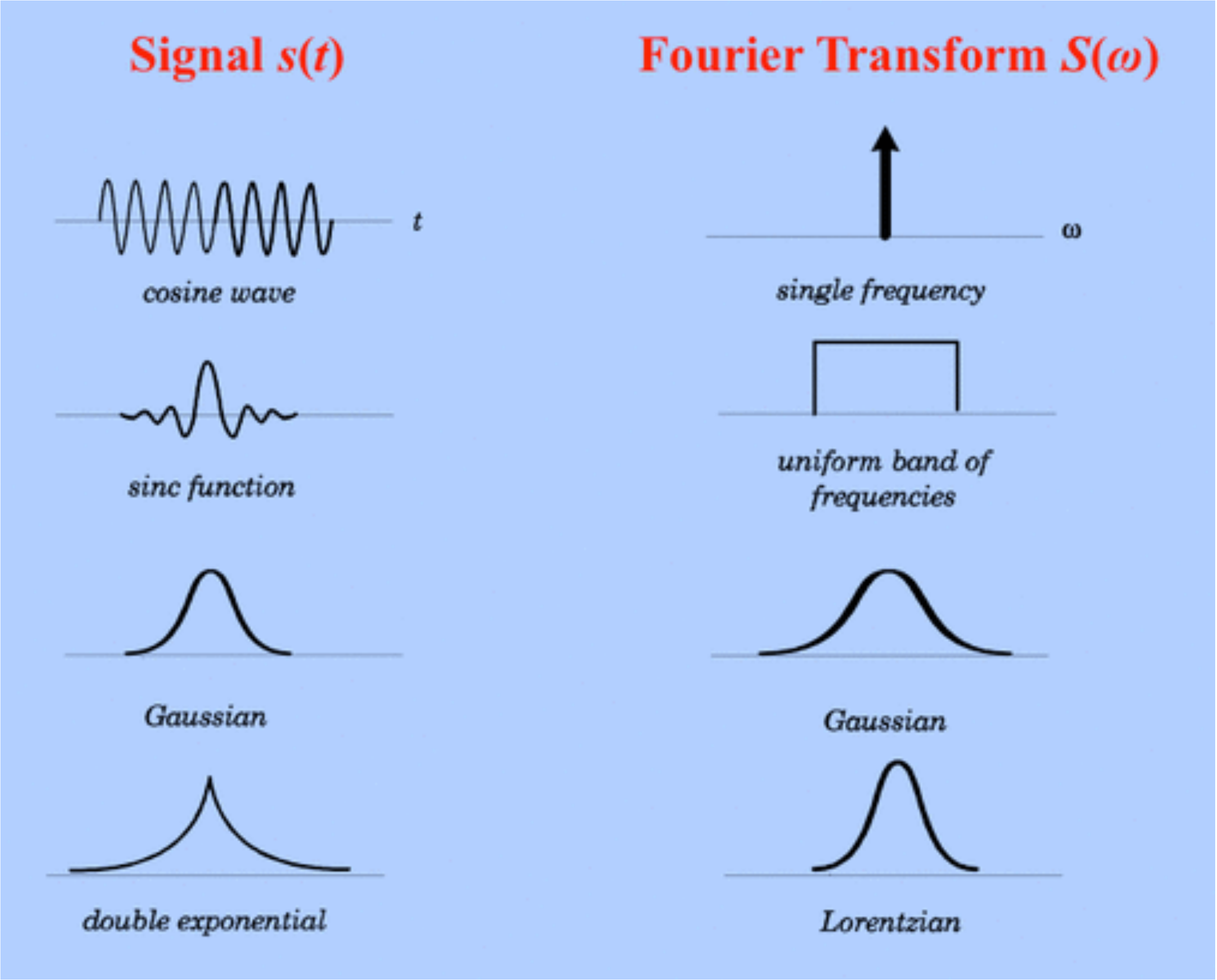
6. Kaj je recipročni prostor?

Analogija: zvočni posnetek in spektrogram





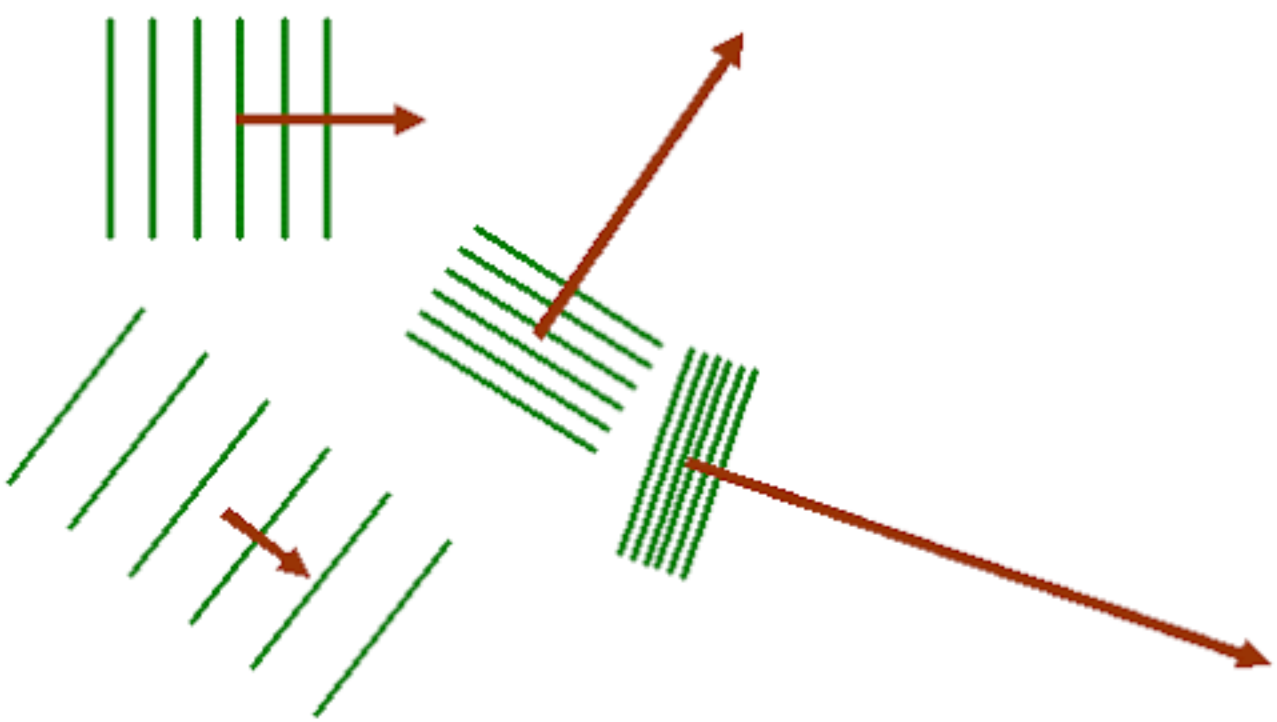
Fourierova transformacija: $\omega \leftrightarrow t$


Signal $s(t)$
Fourier Transform $S(\omega)$
t
ω
cosine wave
single frequency
sinc function
uniform band of frequencies
Gaussian
Gaussian
double exponential
Lorentzian

realni prostor ↔ recipročni prostor $\quad x \leftrightarrow k$

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

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

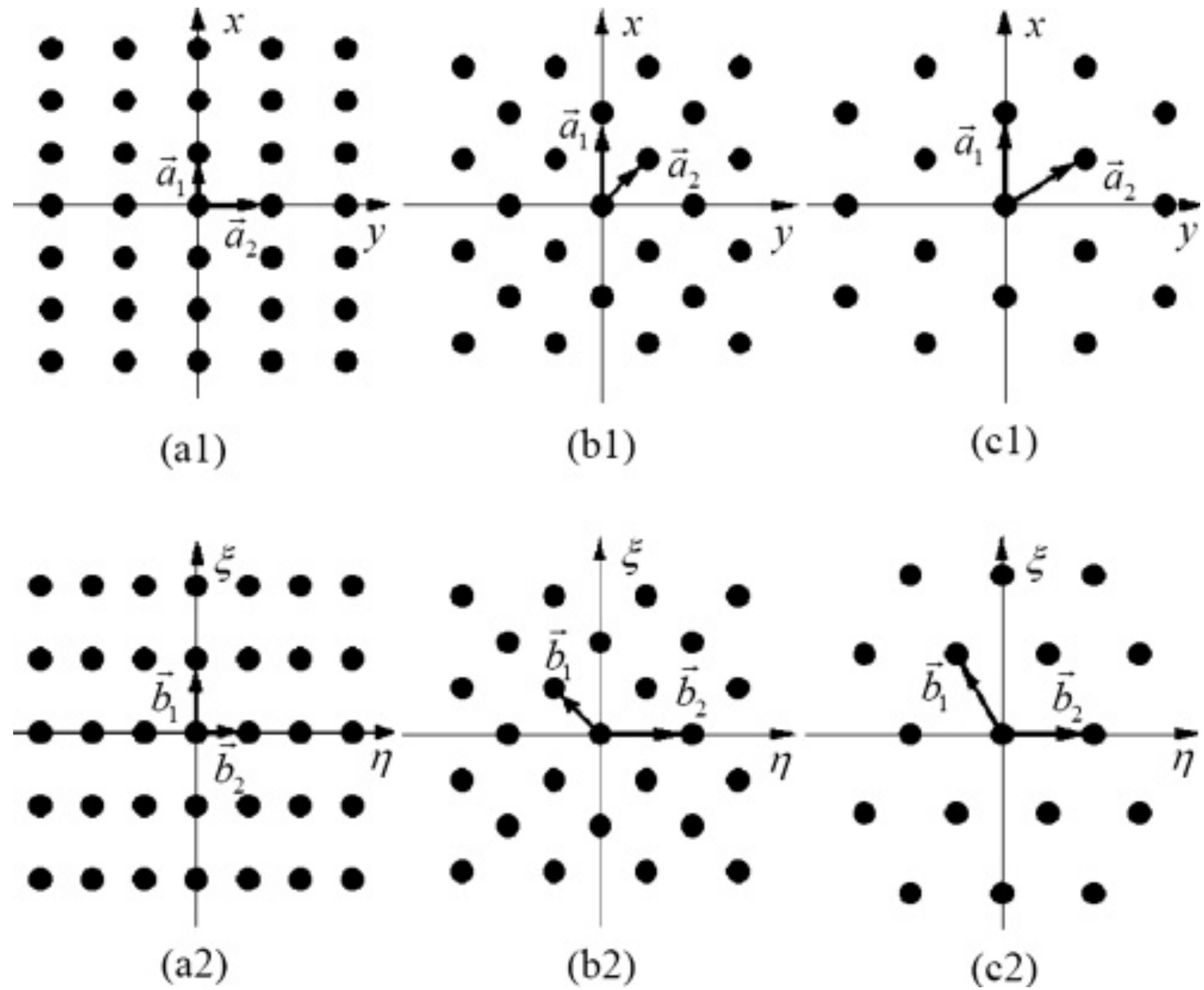


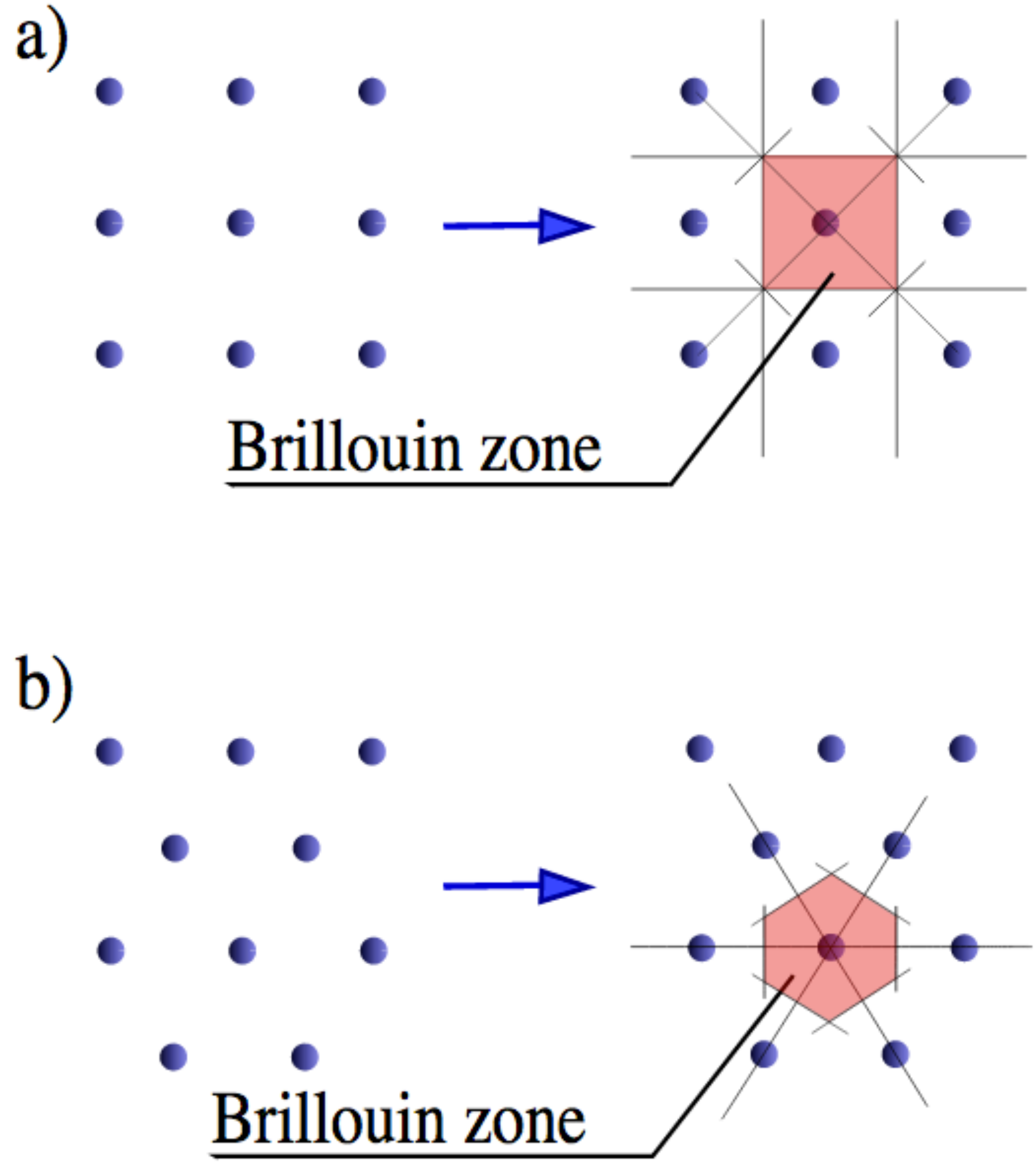
Recipročni mreža

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

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

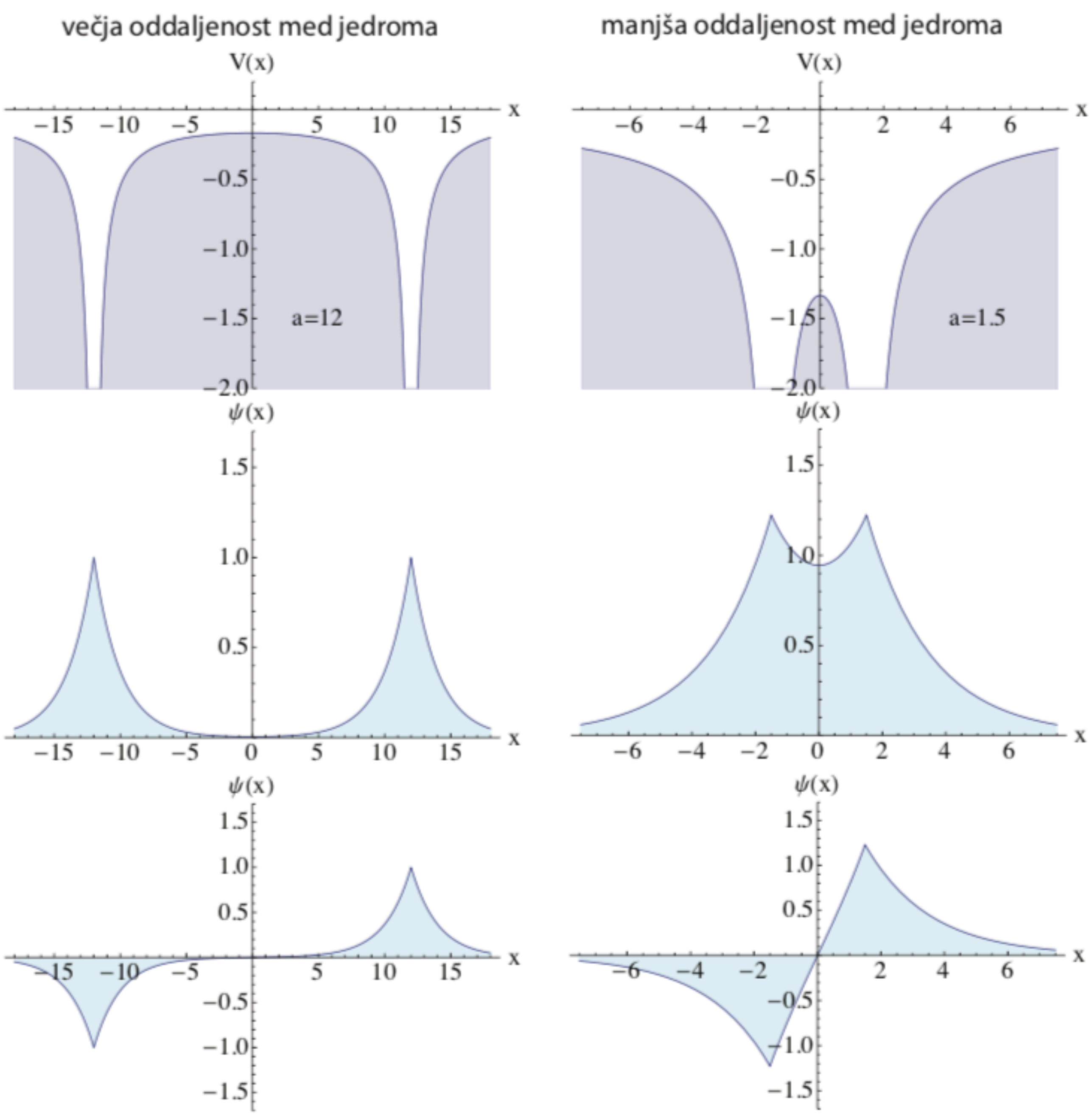
$$\mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{V_{\text{celica}}}$$




a)
Brillouin zone
b)
Brillouin zone

7. Kaj je elektronski pas?
V čem se razlikujejo kovine in izolatorji?

N=2

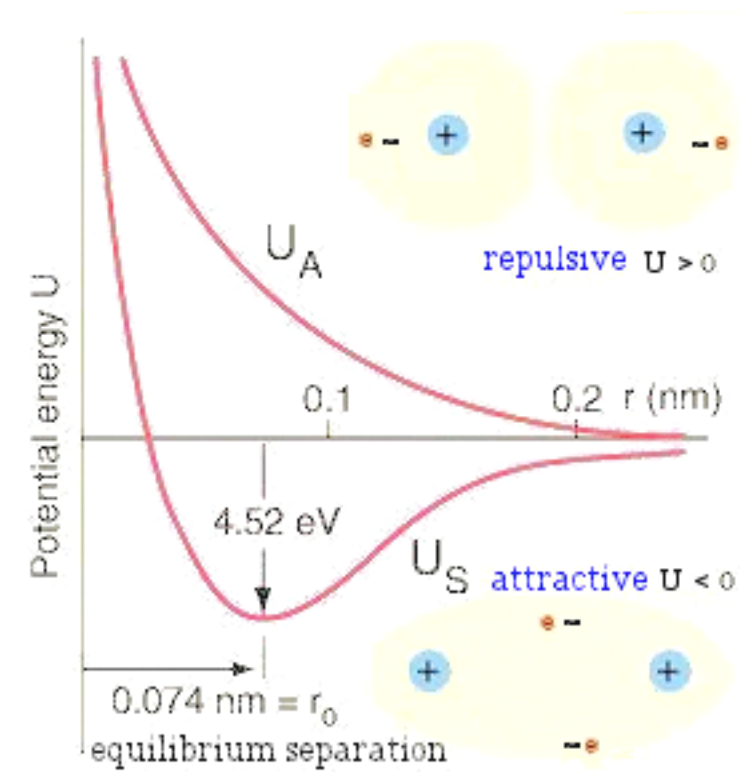


$$\psi_{\text{soda}}(\mathbf{r}) = \frac{1}{\sqrt{2}}\left[\psi(\mathbf{r}-\mathbf{r}_A) + \psi(\mathbf{r}-\mathbf{r}_B)\right]$$

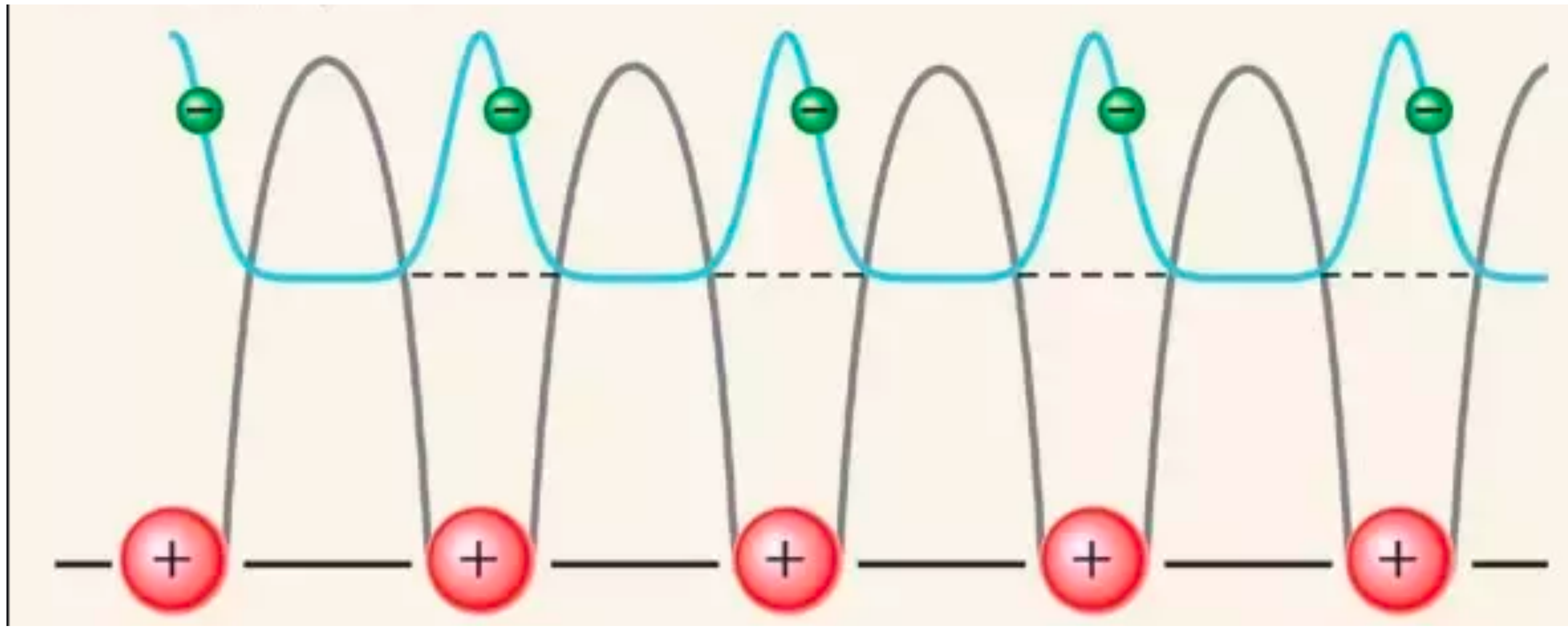
$$\psi_{\text{liha}}(\mathbf{r}) = \frac{1}{\sqrt{2}}\left[\psi(\mathbf{r}-\mathbf{r}_A) - \psi(\mathbf{r}-\mathbf{r}_B)\right]$$

soda kombinacija

liha kombinacija



N velik



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

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

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

$$H = \sum_j \epsilon \left|j\right\rangle \left\langle j\right| - t \left(\left|j\right\rangle \left\langle j+1\right| + \left|j\right\rangle \left\langle j-1\right|\right) \qquad \left|\psi_k\right\rangle = \sum_j \mathrm{e}^{ikja} \left|j\right\rangle$$

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

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

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

```
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 × 72]
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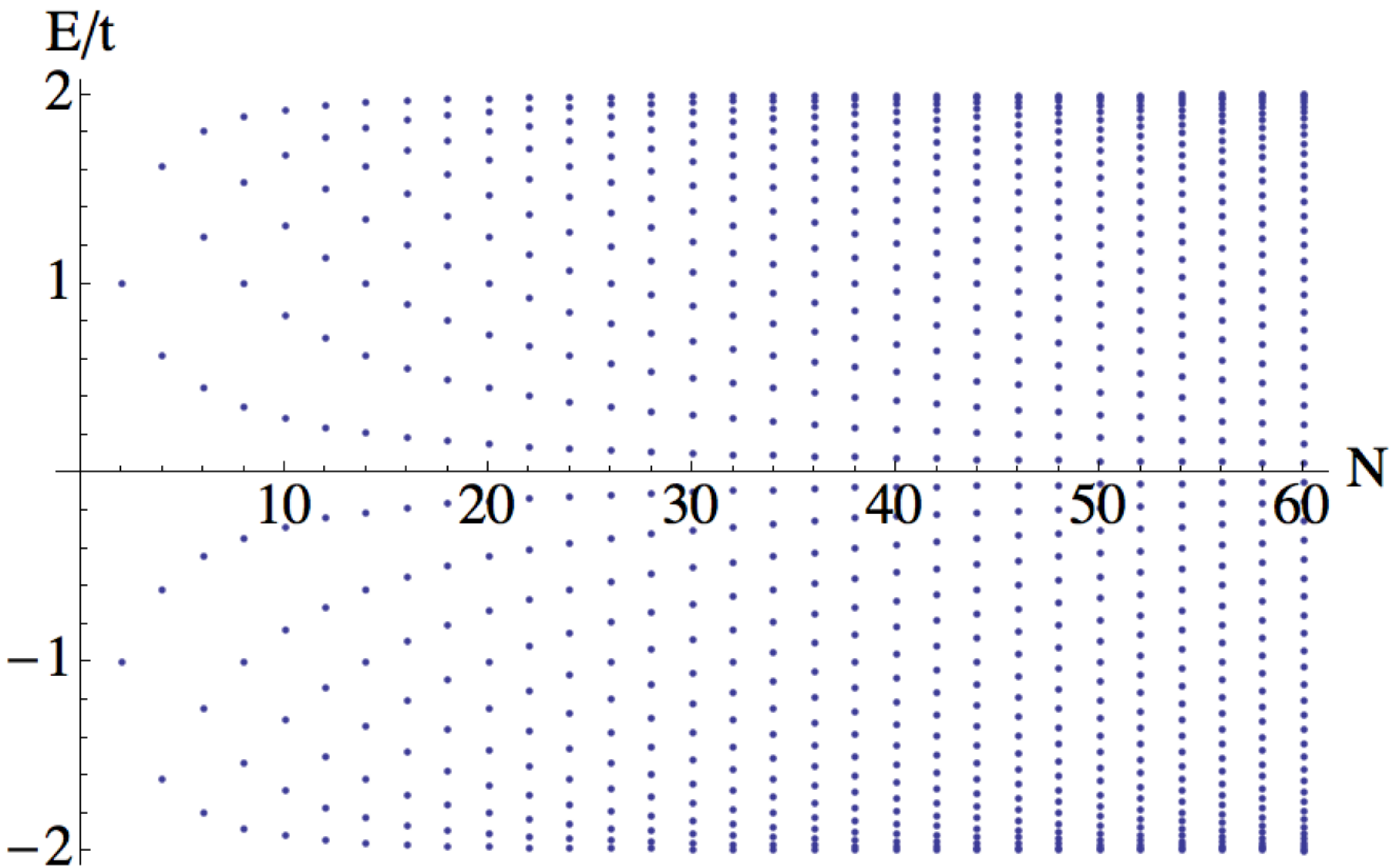
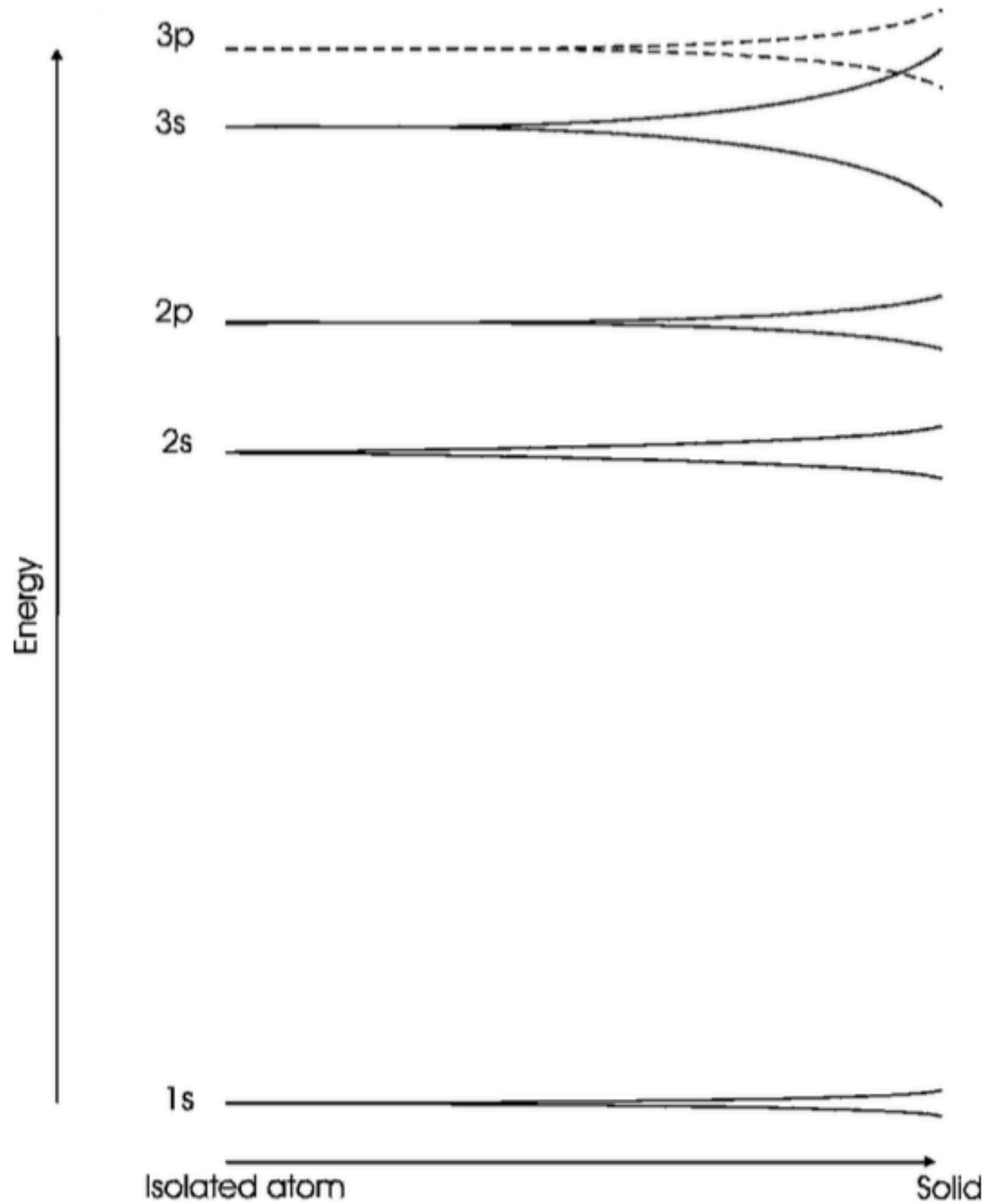
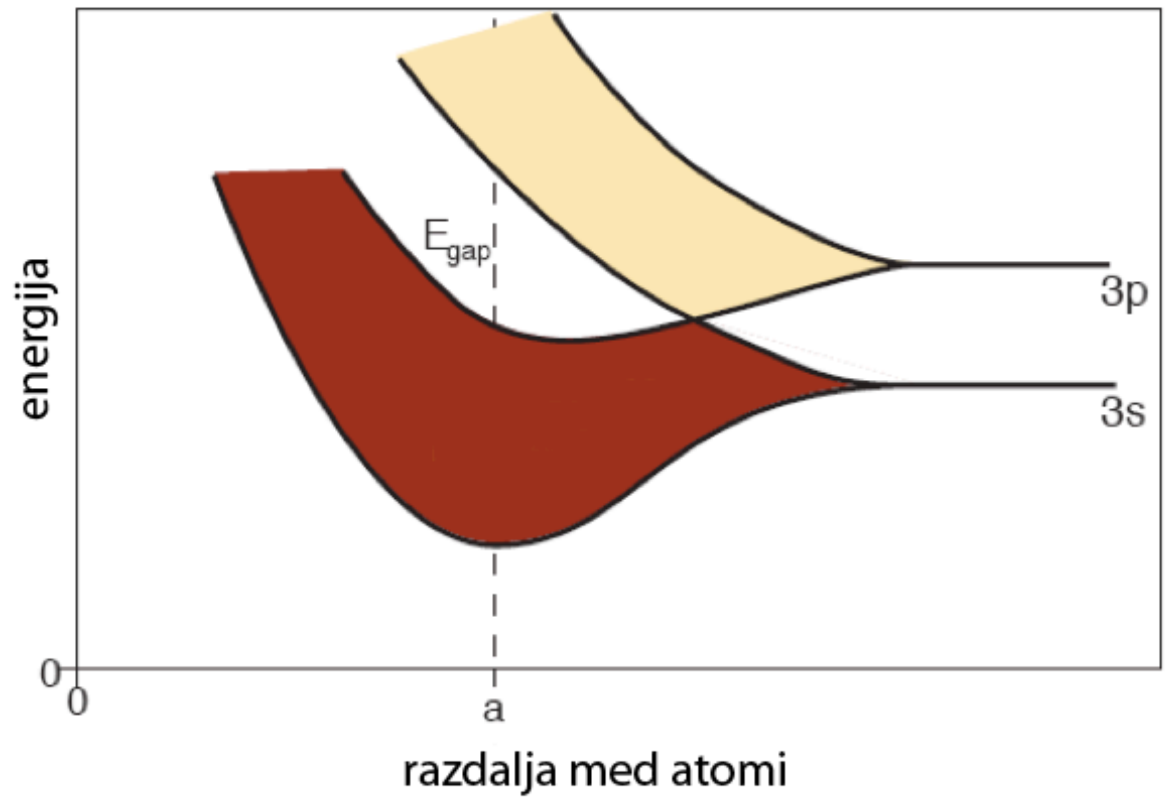
Out[21]=

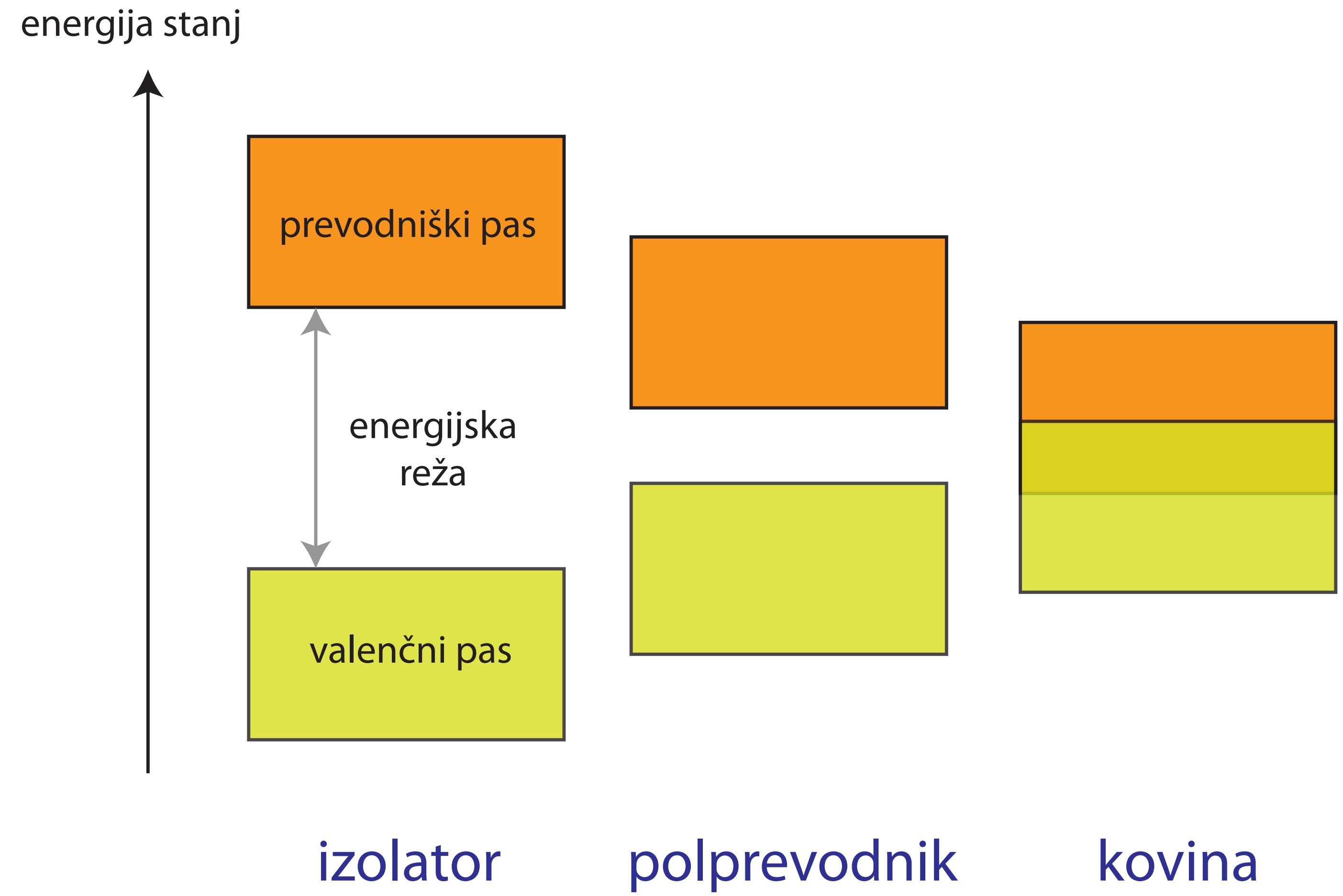




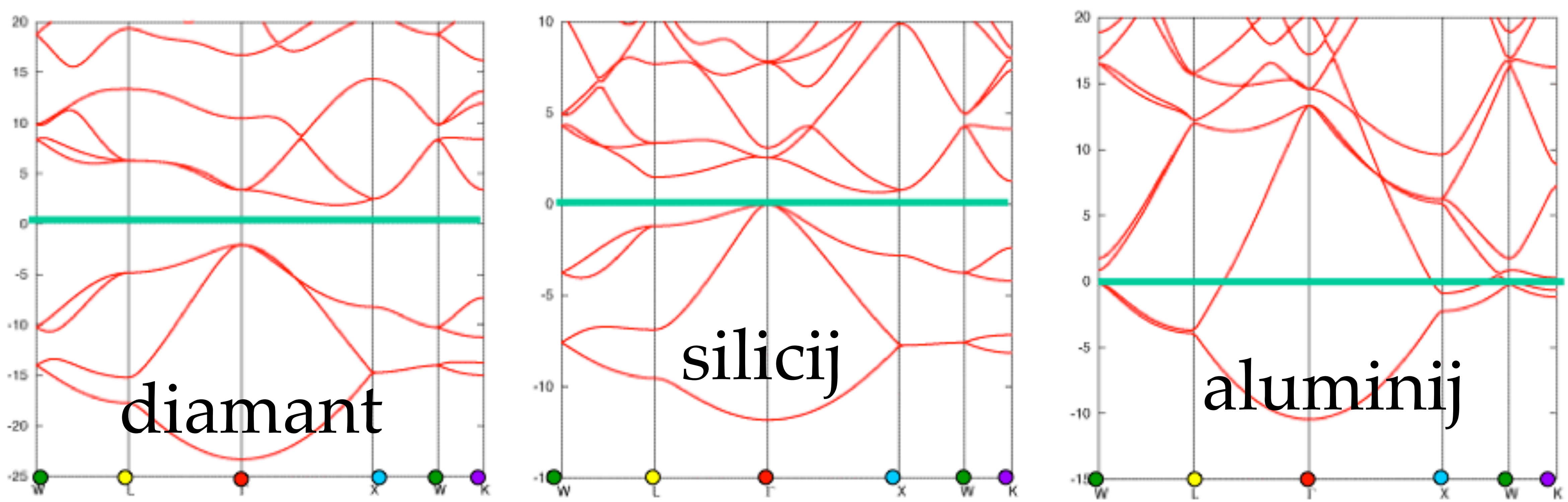
Mg

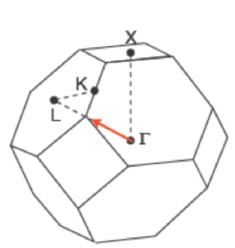
TEORIJA PASOV



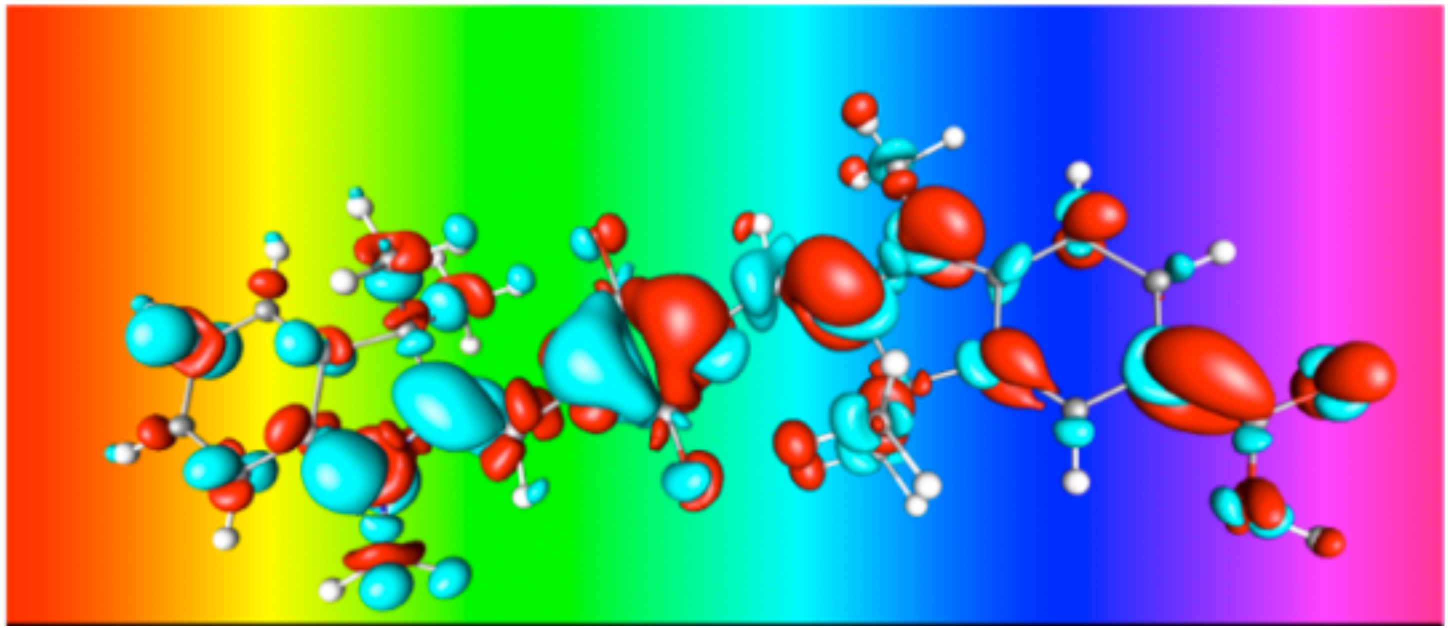


pasovna struktura





Računska kemija



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/
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  ntyp = 1,
  ecutwfc = 20
/
&electrons
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/
ATOMIC_SPECIES
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ATOMIC_POSITIONS (alat)
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K_POINTS (automatic)
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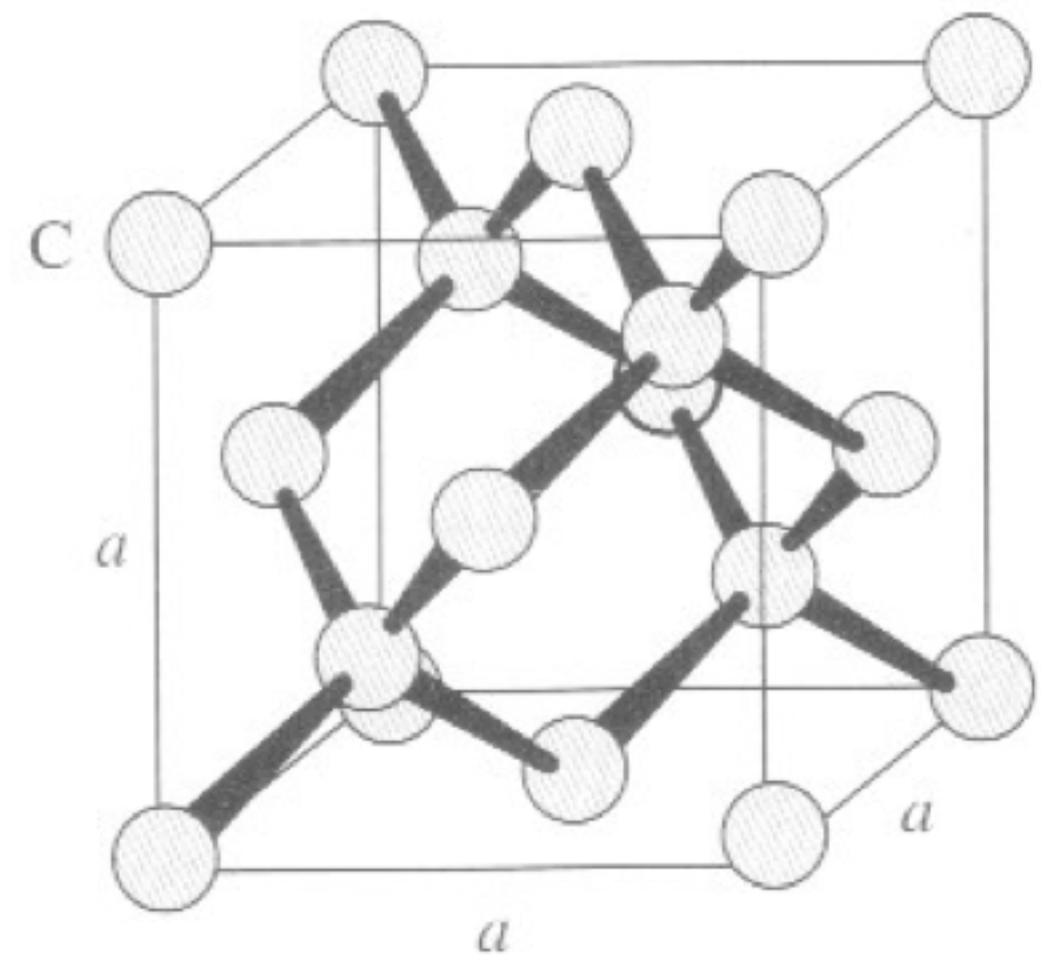
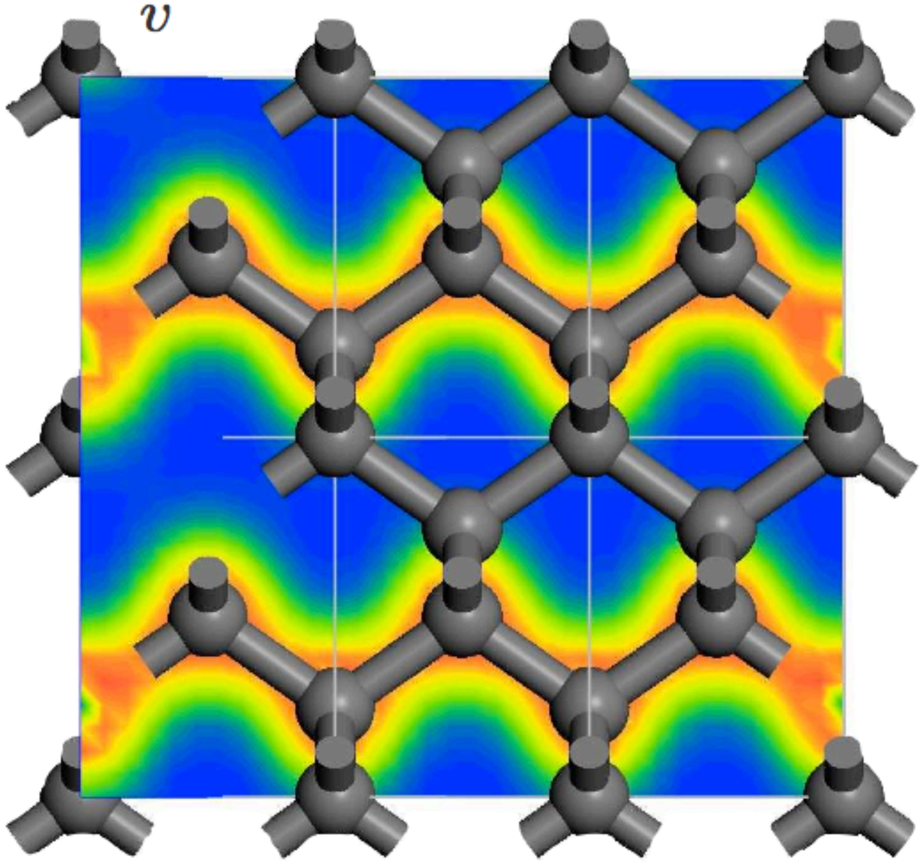
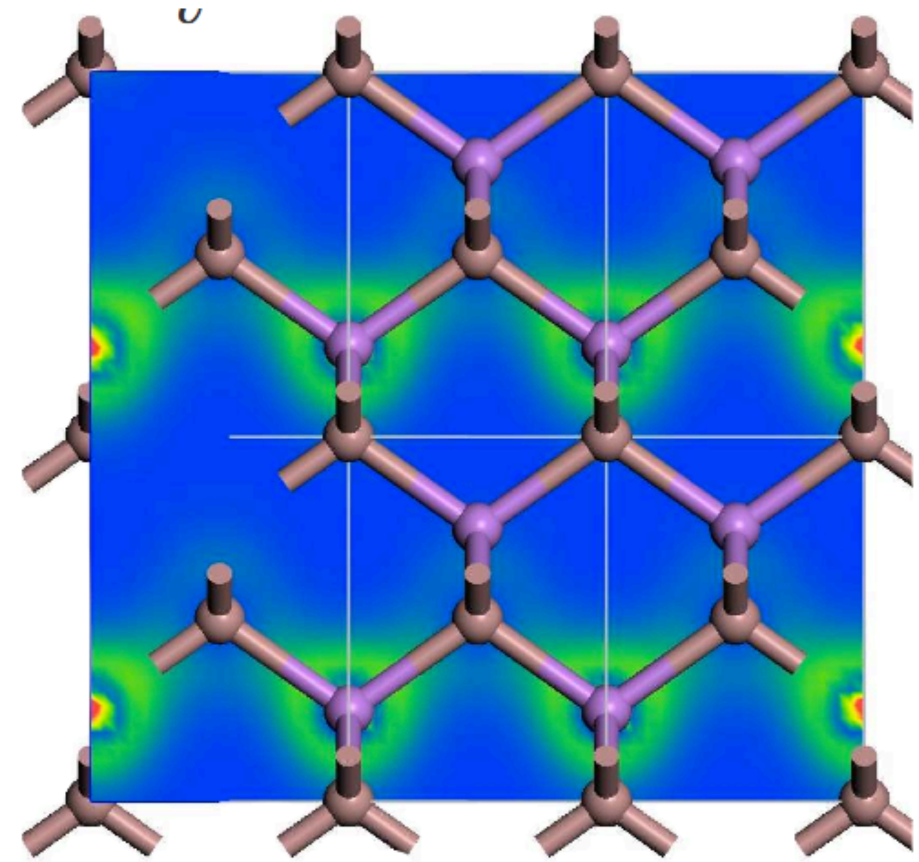




diamond



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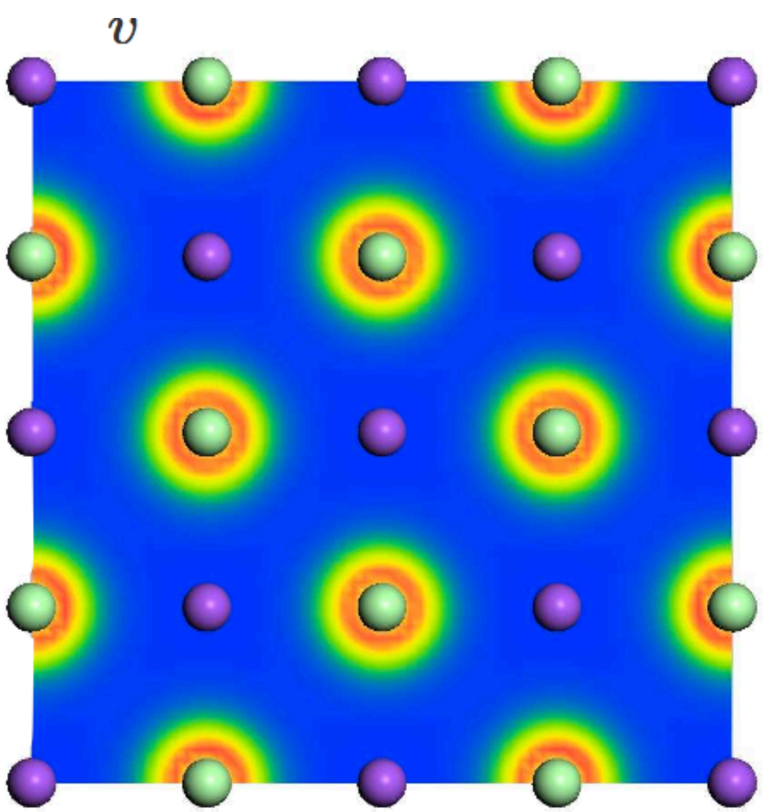

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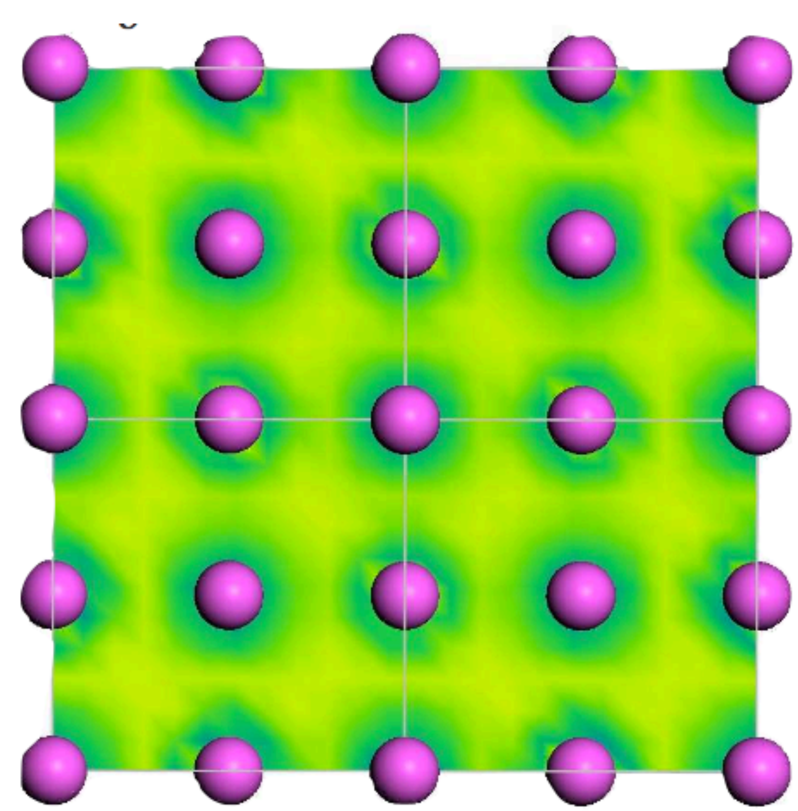
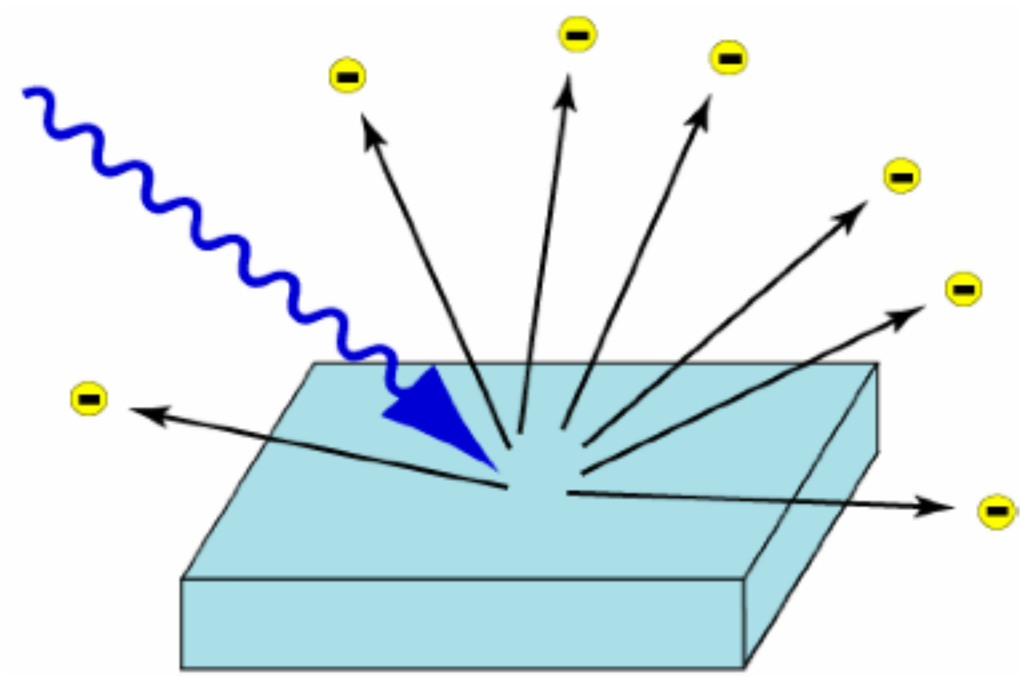
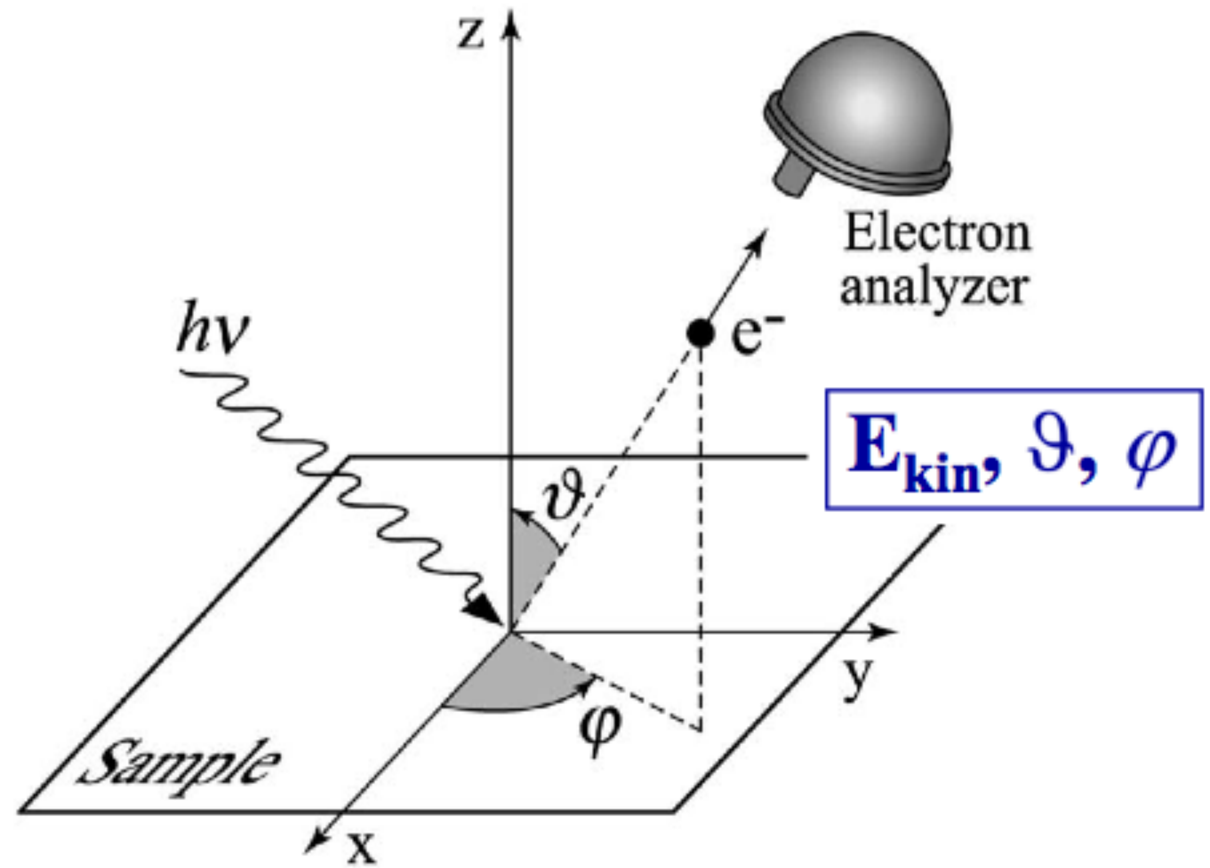


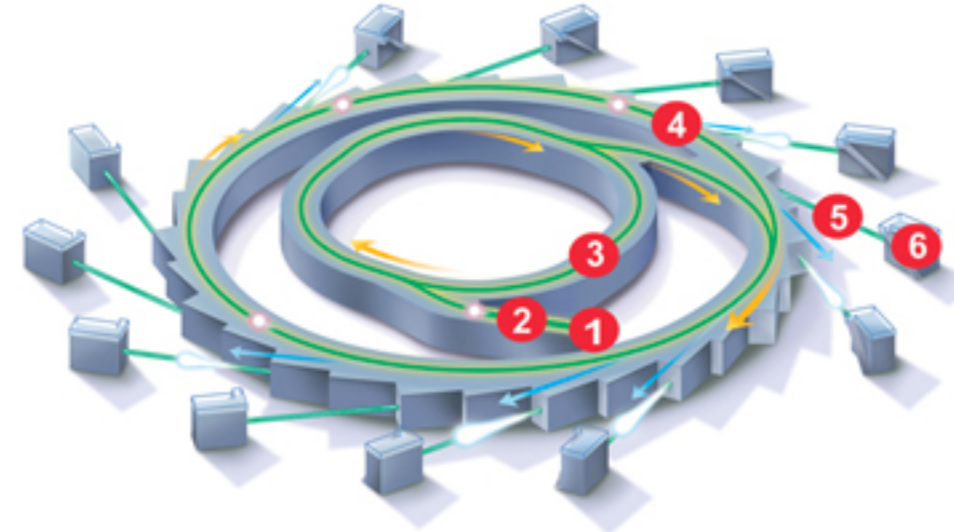
Aluminum

ARPES





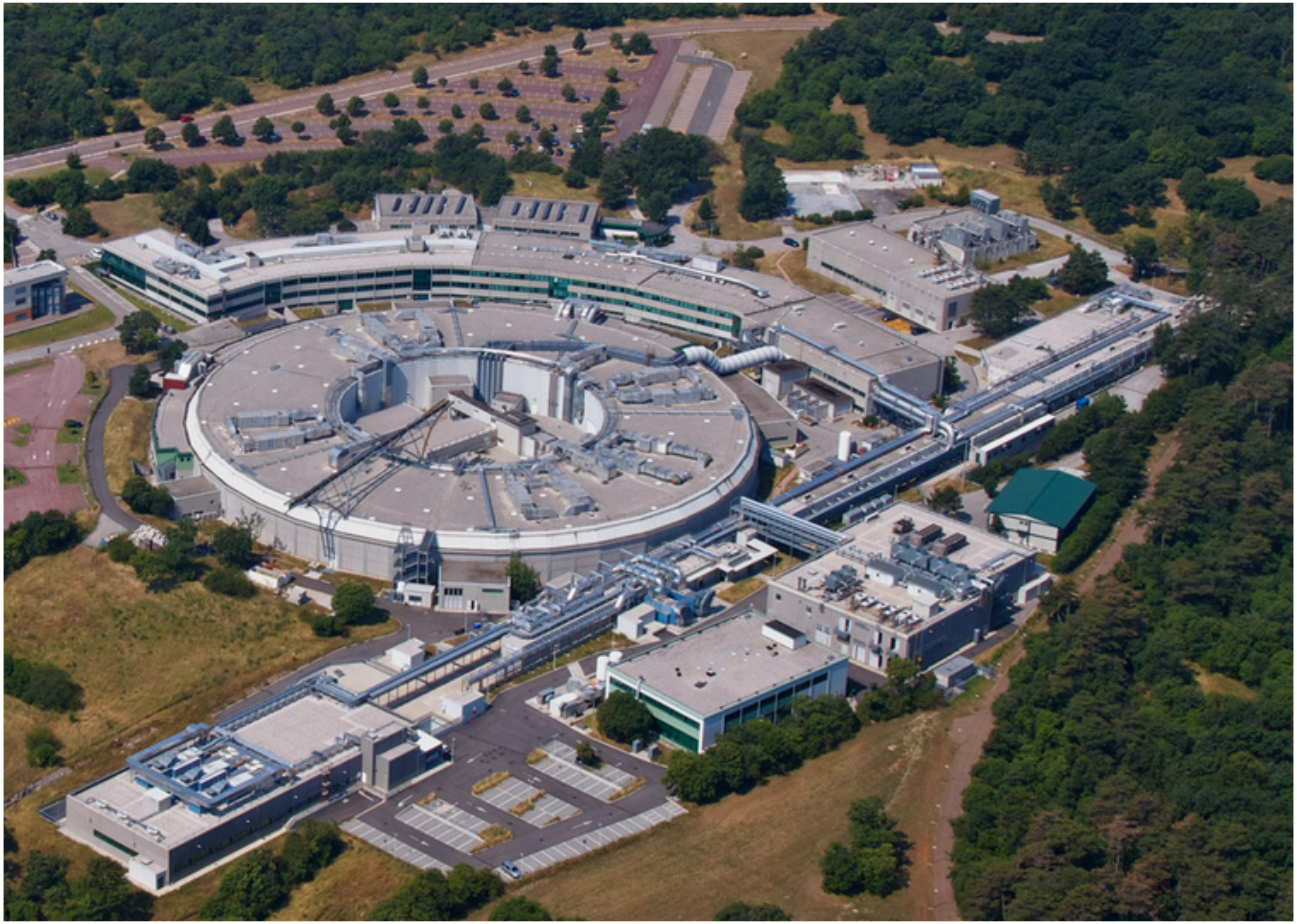
z
Electron
analyzer
e^-
$h\nu$
$E_{kin}, \vartheta, \varphi$
ϑ
y
φ
Sample
x



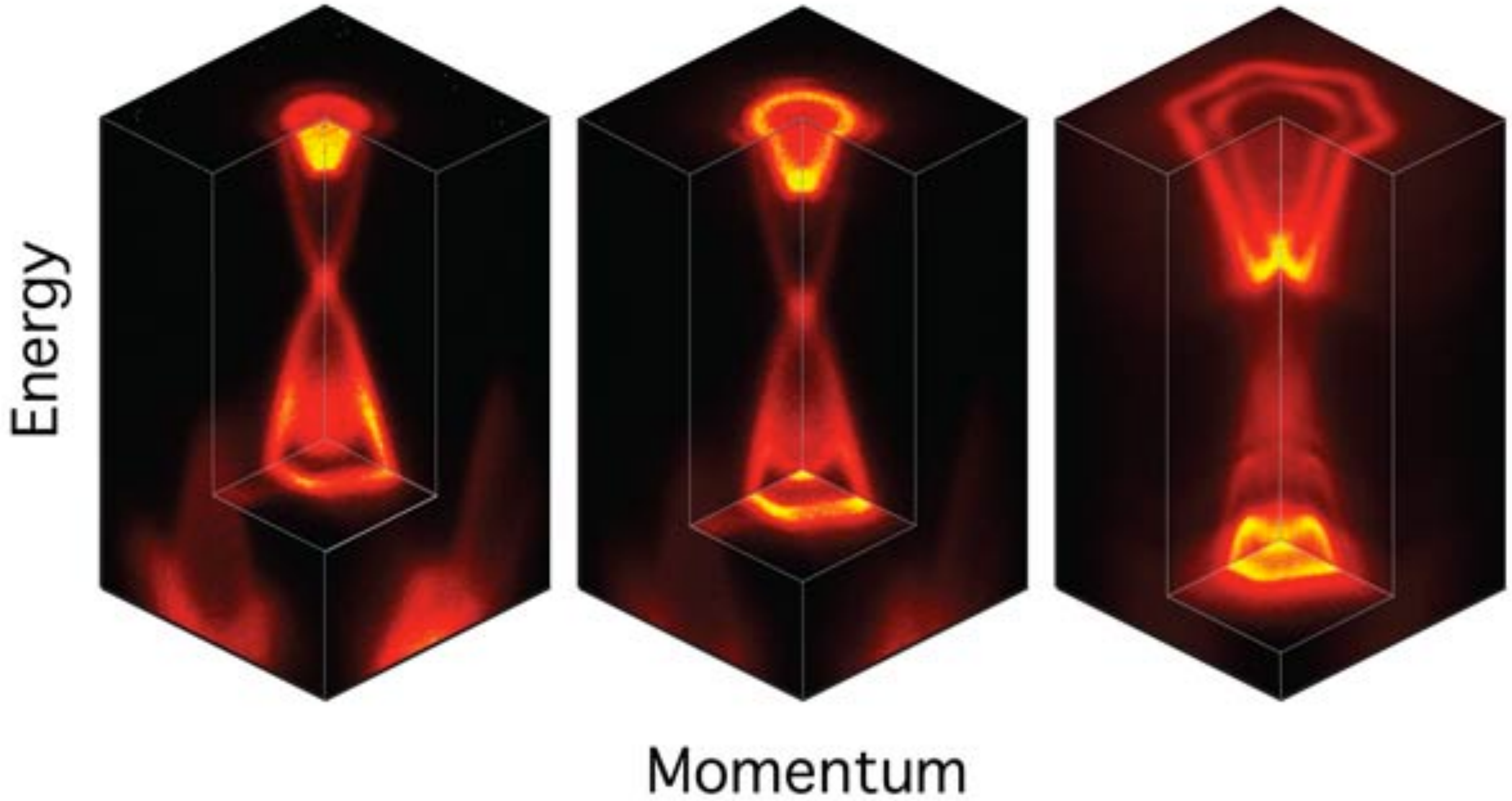
Diamond (UK, blizu Oxforda)

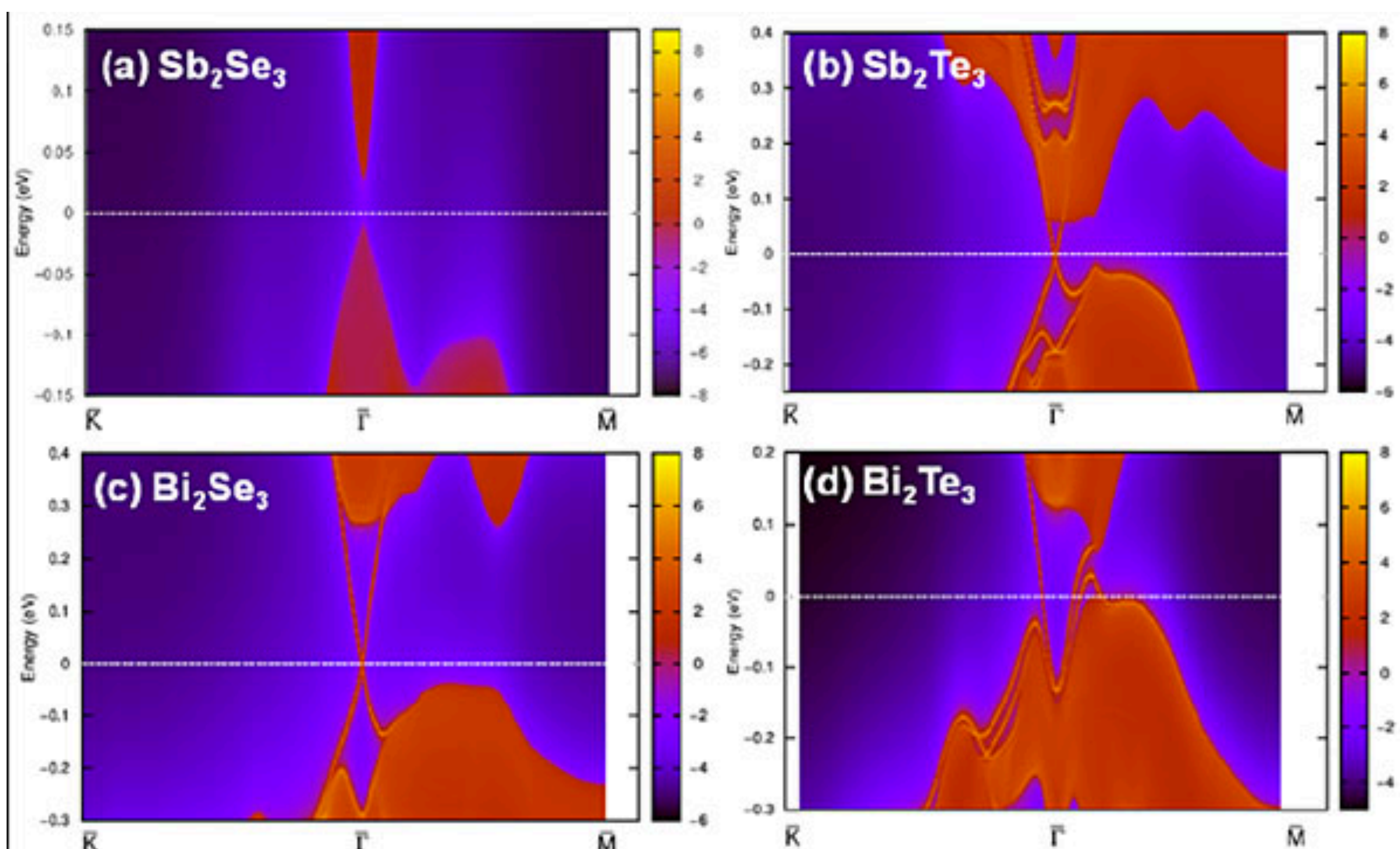
Peking (2018)

Elettra, Bazovica



Elettra, Bazovica pri Trstu


Energy
Momentum


(a) Sb2Se3
(b) Sb2Te3
(c) Bi2Se3
(d) Bi2Te3
Energy (eV)
K̄
Γ̄
M̄