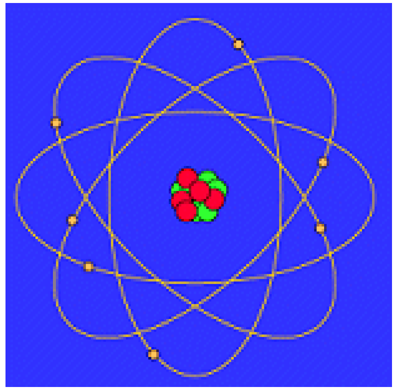
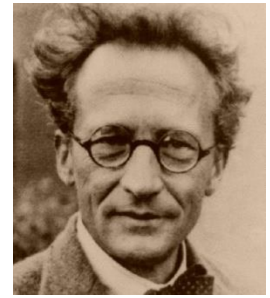
TEMA 5

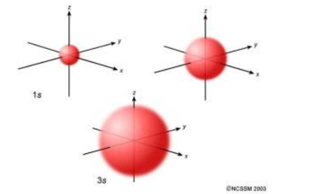
Principios de Cristaloquímica

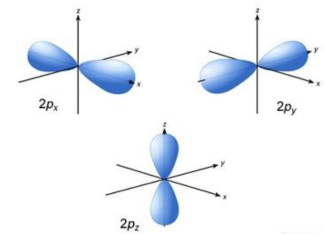
Átomo de Bohr



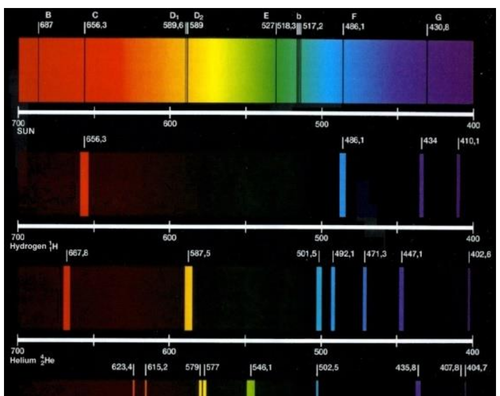
Átomo de Schrödinger

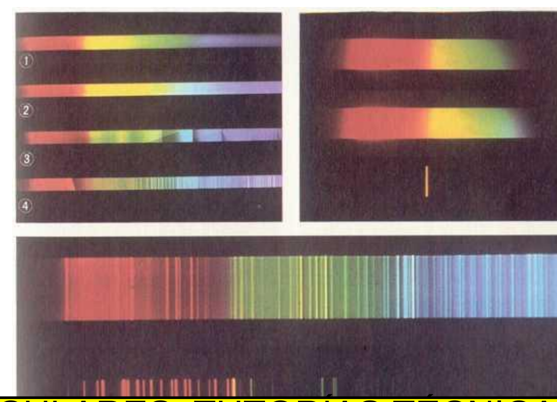


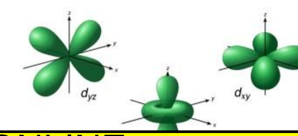




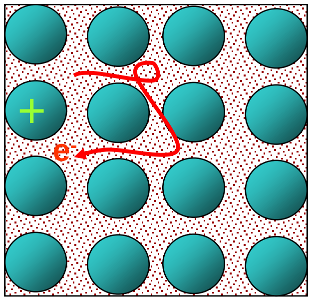
Espectros atómicos



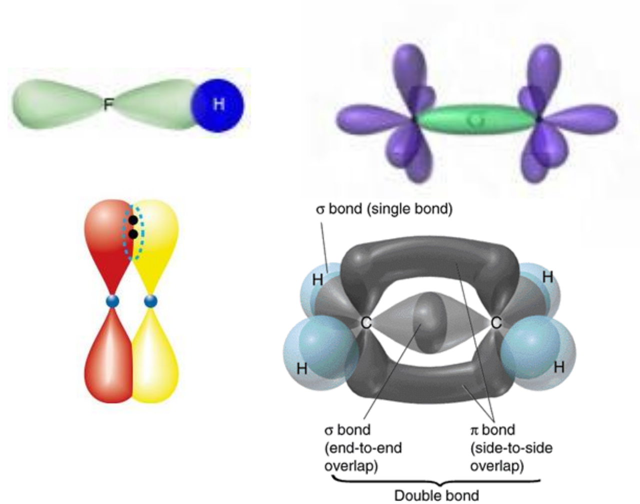




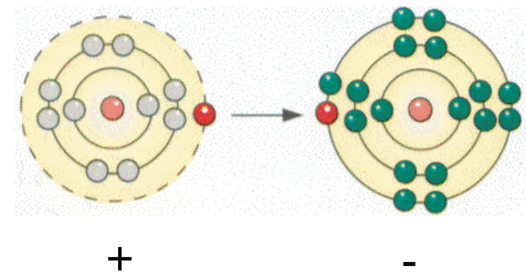
Enlace Metálico



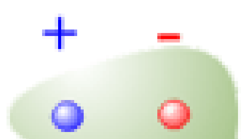
Enlace covalente



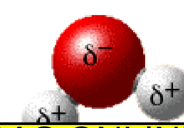
Enlace iónico



Enlace de van der Waals

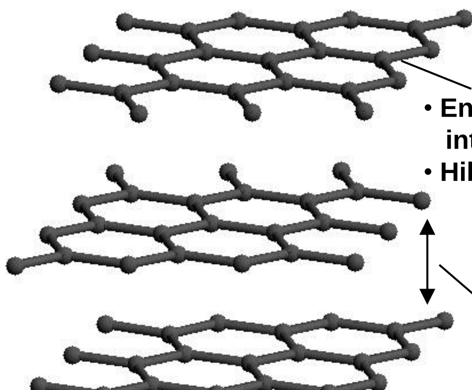


Enlace por puente de hidrógeno



Combinación de enlaces

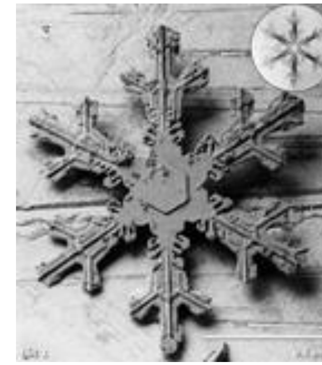
Grafito. C

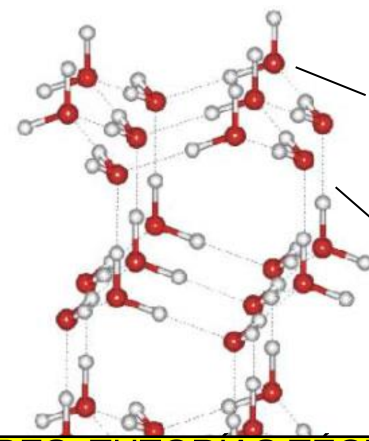


- **Enlace covalente (fuerte) intracapa**
- **Hibridación sp2**

- **Fuerzas de van der Waals (débiles)**

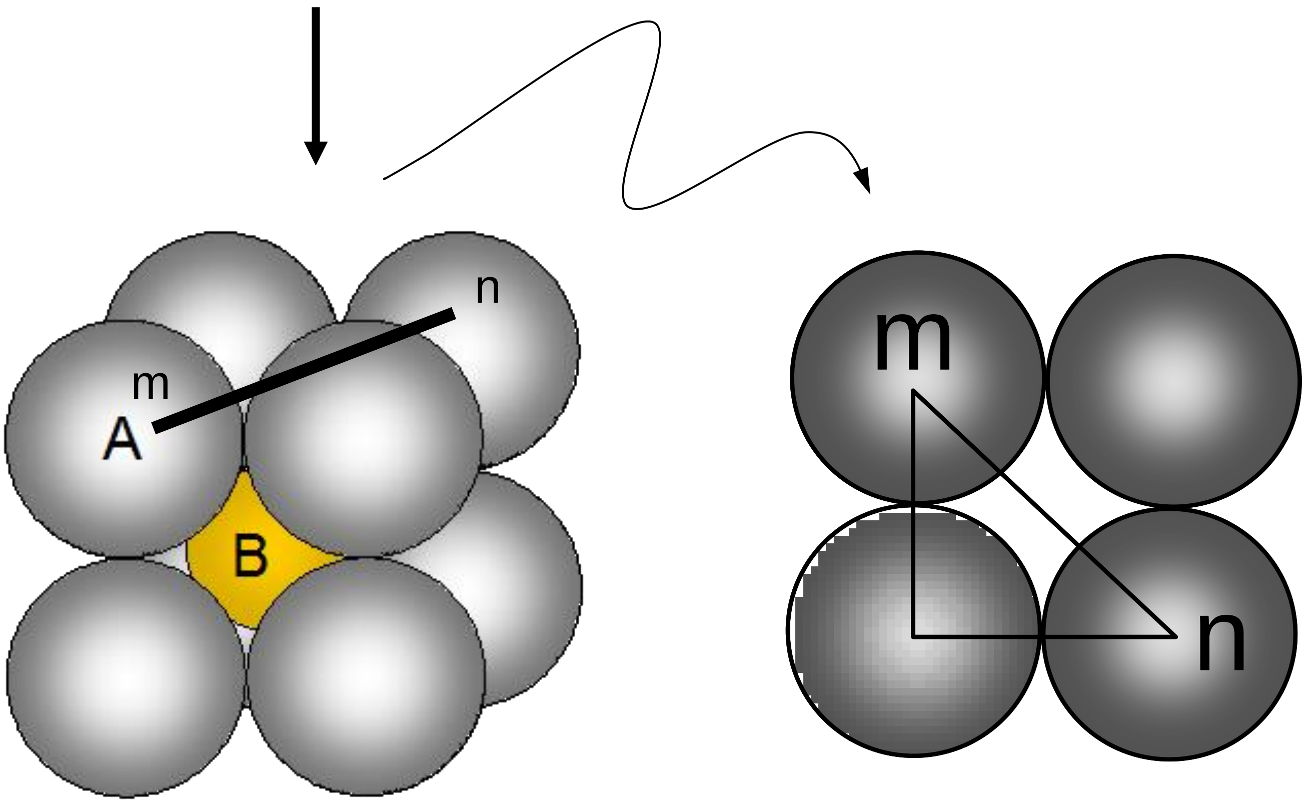
Hielo. H_2O





- **Enlace covalente (fuerte) entre el oxígeno y dos hidrógenos**

- **Enlaces de puente de hidrogeno (débiles)**


n
m
A
B
m
n

Esquemas de coordinación

Relación $R_{B/}R_A$ mínima	NC	Geometría
< 0,155	2	lineal
0,155	3	triangular
0,255	4	tetraédrica
0,414	6	octaédrica
0,732	8	cúbica

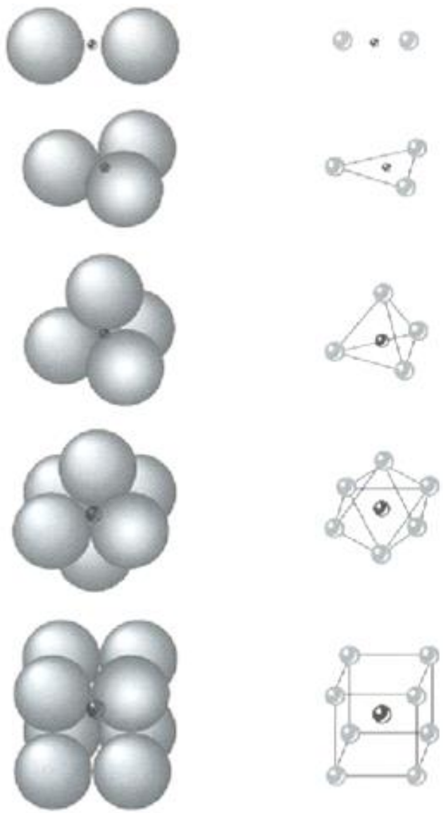
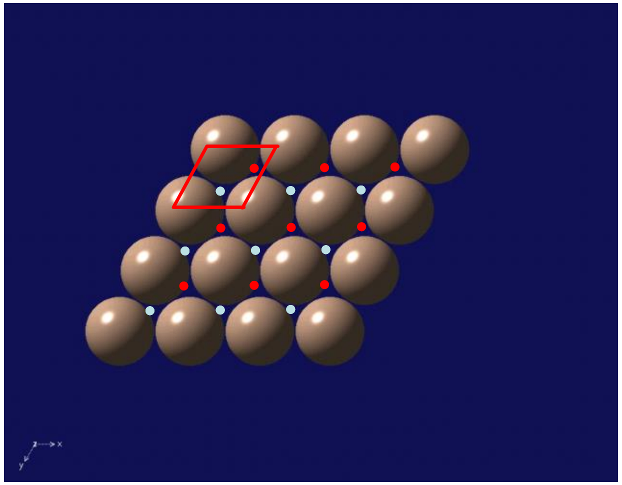


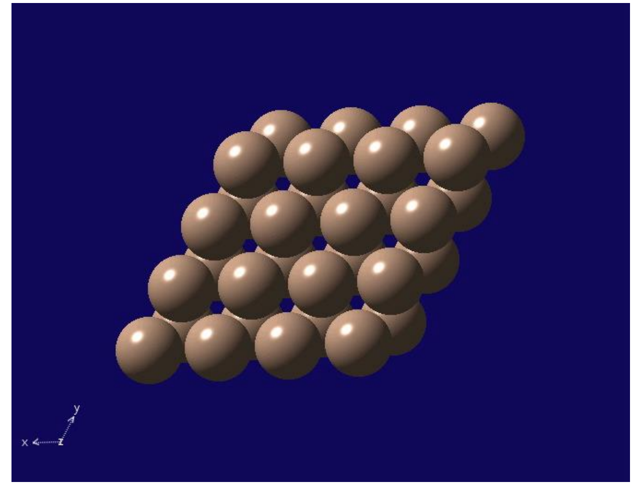
Tabla de electronegatividades

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
H																	He
2.1																	-
Li	Be											B	C	N	O	F	Ne
1.0	1.5											2.0	2.5	3.05	3.5	4.0	-
Na	Mg											Al	Si	P	S	Cl	Ar
0.9	1.2											1.61	1.9	2.19	2.5	3.0	-
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
0.8	1.0	1.3	1.5	1.6	1.6	1.5	1.8	1.8	2.8	1.9	1.65	1.81	2.01	2.0	2.4	2.8	-
		http://www.fortunecity.com/campus/dawson/196															
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
0.8	1.0	1.2	1.4	1.6	1.8	1.9	2.2	2.28	2.2	1.9	1.9	1.78	1.8	1.9	2.1	2.5	-
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
0.79	1.02	1.17	1.3	1.54	1.7	1.9	2.2	2.2	2.7	2.4	1.9	1.8	1.8	1.9	2.0	2.2	-
Fr	Ra	Ac															
0.7	0.9	1.1															
		Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu		

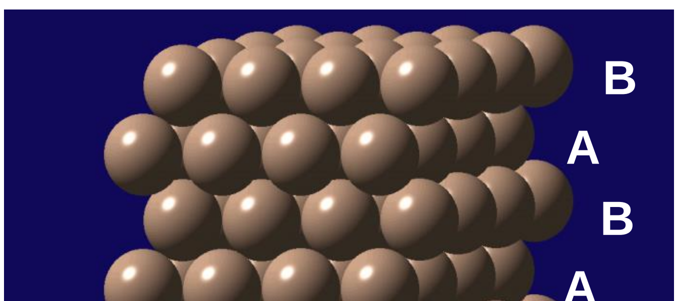
EMPAQUETADOS COMPACTOS



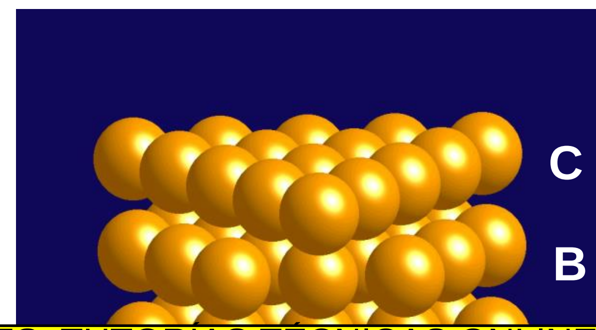
Capa de empaquetamiento hexagonal compacto



Apilamiento de la segunda capa

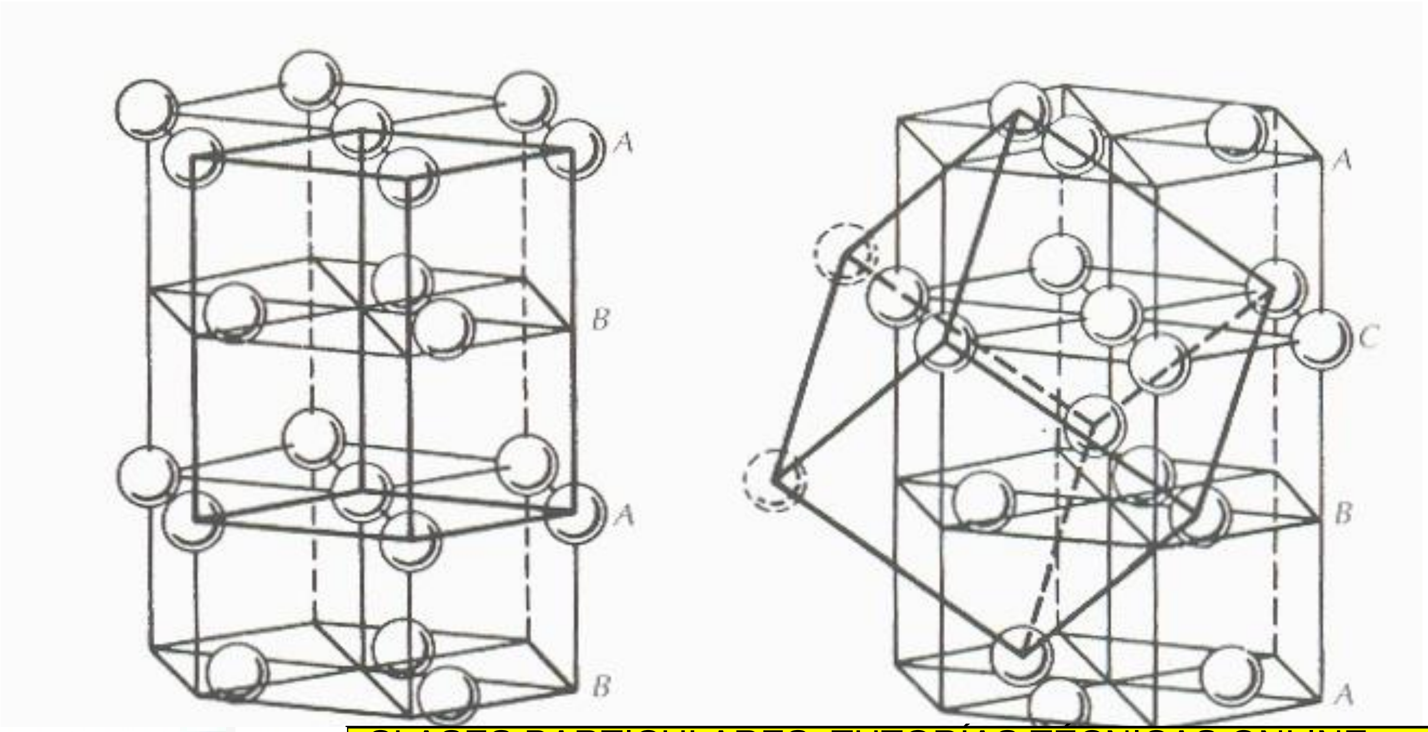


Hexagonal compacto

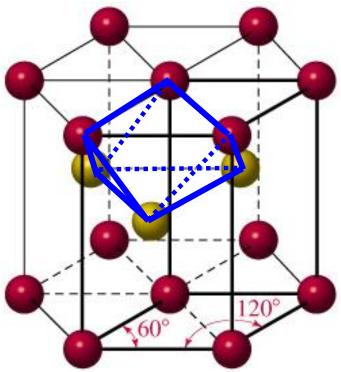


Cúbico compacto

hcp   ccp

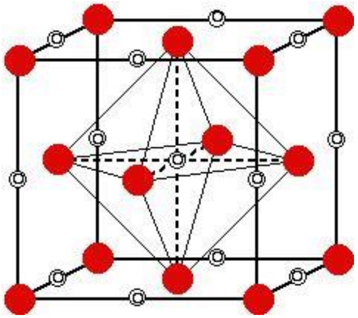


HCP

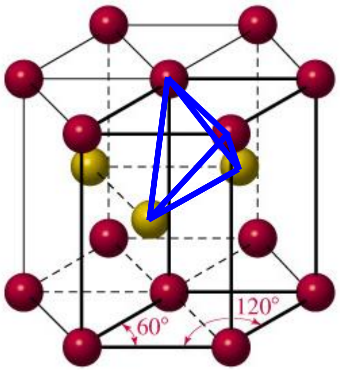


4 posiciones octaédricas

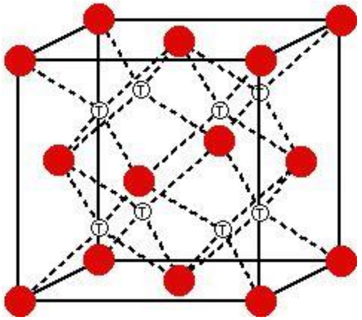
CCP



4 posiciones octaédricas

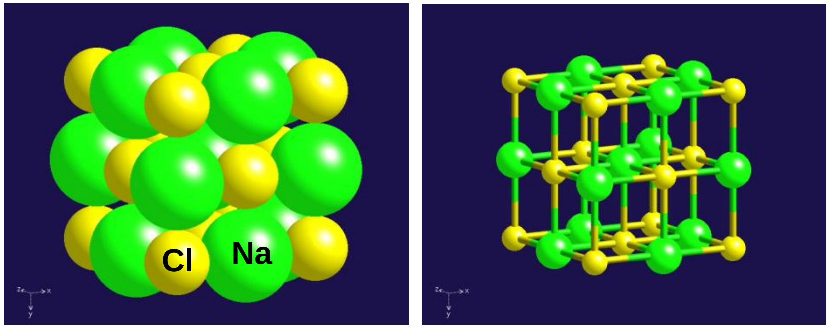


8 posiciones tetraédricas

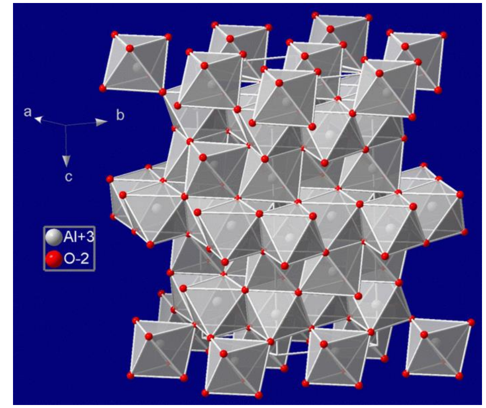


8 posiciones tetraédricas

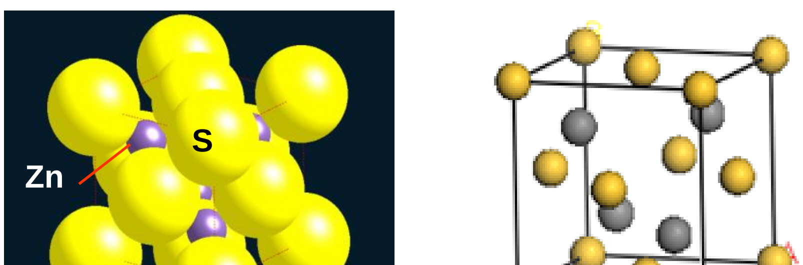
Estructura de la halita (NaCl)



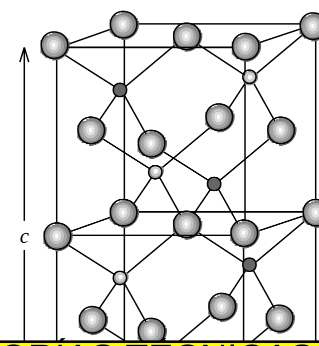
Estructura del corindón (Al_2O_3), el hematites, Fe_2O_3 la ilmenita Fe_2TiO_3



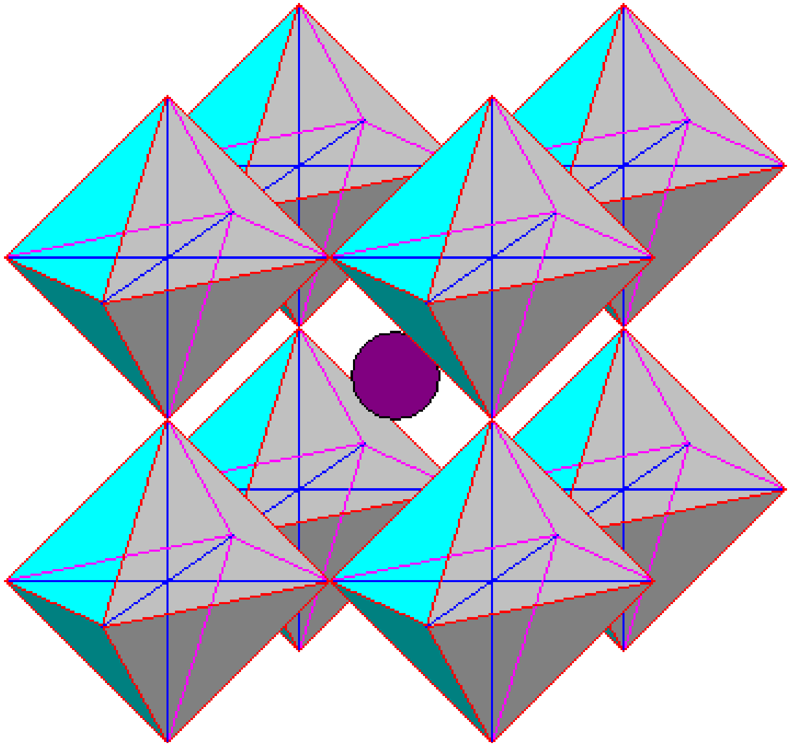
Estructura de la blenda (ZnS)

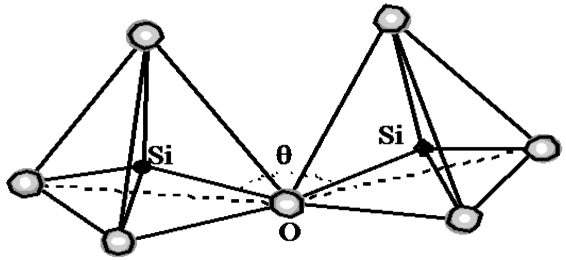


Estructura de la calcopirita (CuFeS)

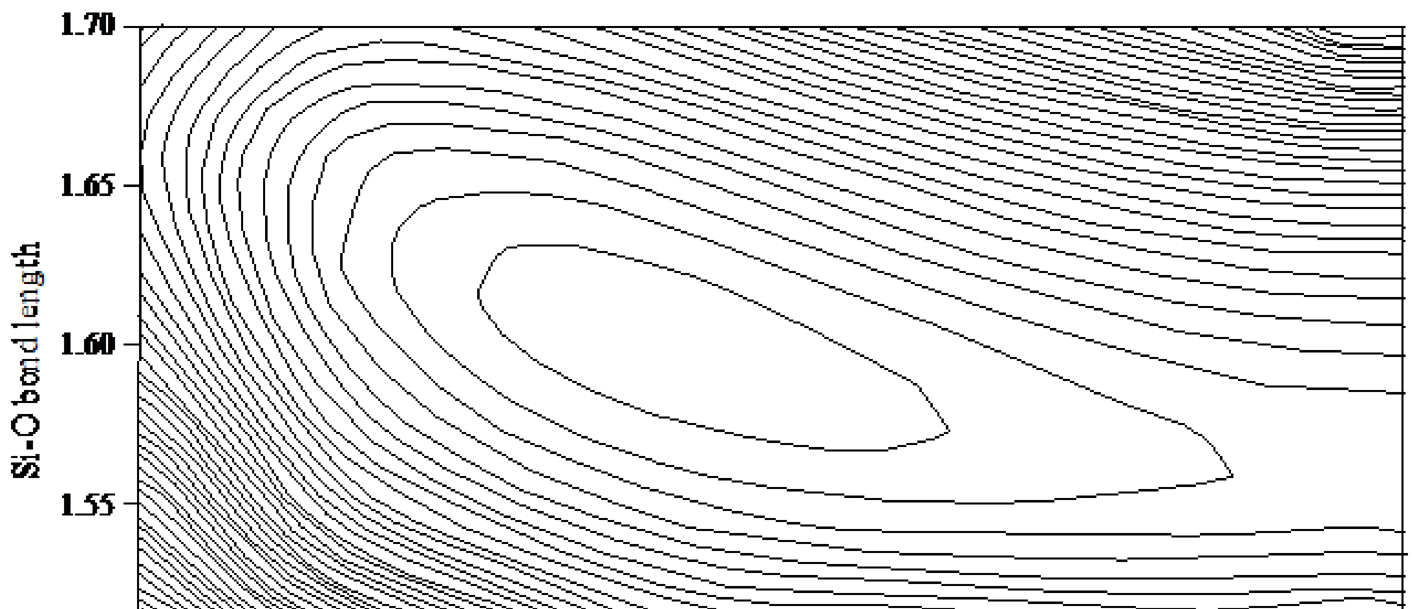


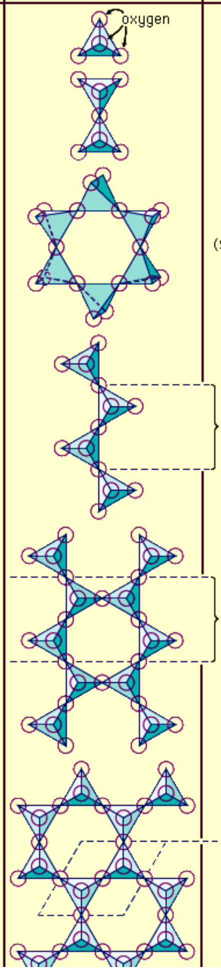
Estructura de la Perovskita ($CaTiO_3$)





$[Si_2O_7]^{6-}$





class	arrangement of SiO_4 tetrahedrons (central Si^{4+} not shown)	unit composition	mineral example
Nesosilicates		$(SiO_4)^{4-}$	Olivine, $(Mg, Fe)_2SiO_4$
Sorosilicates		$(Si_2O_7)^{6-}$	Hemimorphite, $Zn_4Si_2O_7(OH)_2 \cdot H_2O$
Cyclosilicates		$(Si_6O_{18})^{12-}$	Beryl, $Be_3Al_2Si_6O_{18}$
Inosilicates (single chain)		$(Si_2O_6)^{4-}$	Pyroxene *e.g.*, enstatite, $MgSiO_3$
Inosilicates (double chain)		$(Si_4O_{11})^{6-}$	Amphibole *e.g.*, anthophyllite, $Mg_7Si_8O_{22}(OH)_2$
Phyllosilicates		$(Si_2O_5)^{2-}$	Mica *e.g.*, phlogopite, $KMg_3(AlSi_3O_{10})(OH)_2$

Unidades estructurales del los silicatos

Nesosilicatos: tetraedros SiO_4. Si:O = 1/4

Sorosilicatos: dos tetraedros unidos por un oxígenos. Si:O = 1:3,5

Ciclosilicatos: anillos de varios tetraedros

Inosilicatos:

Piroxenos: Cadenas sencillas de tetraedros. Si:O =1/3.
Anfíboles: Cadenas dobles de tetraedros. Si:O = 3 y Si:O = 2,5. La relación Si:O total es 1:2,75.

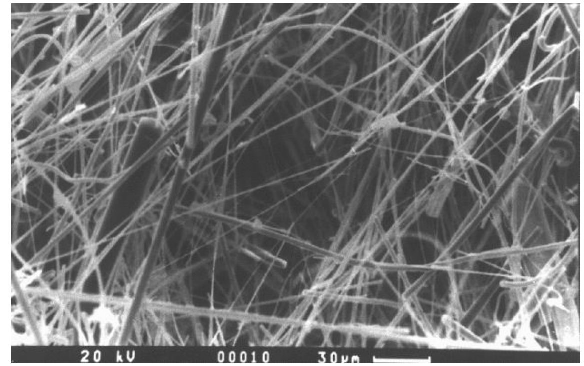
Filosilicatos: láminas con disposición hexagonal de tetraedros Si:O =1:2,5.

Tectosilicatos: armazones tridimensionales de tetraedros.Si:O = 1/2

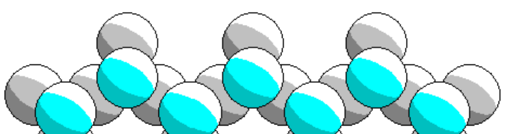
- Los defectos de carga de las unidades estructurales se compensan con la entrada de cationes en las estructuras.

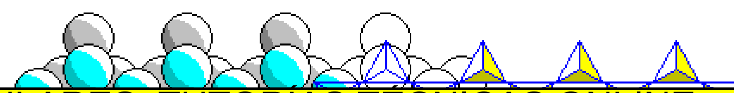
- Las estructura básica de los tectosilicatos no tiene carga. Sin

Anfíboles: asbestos

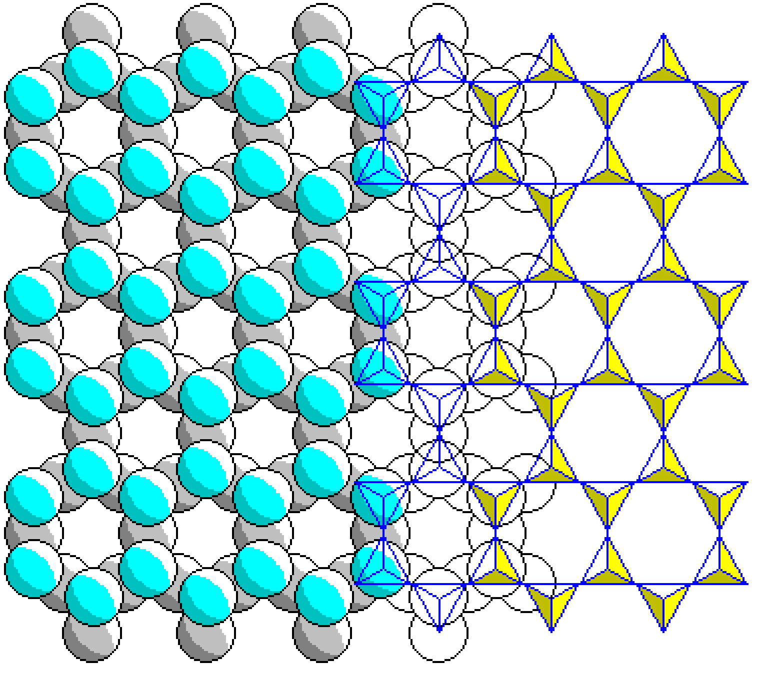


Piroxenos



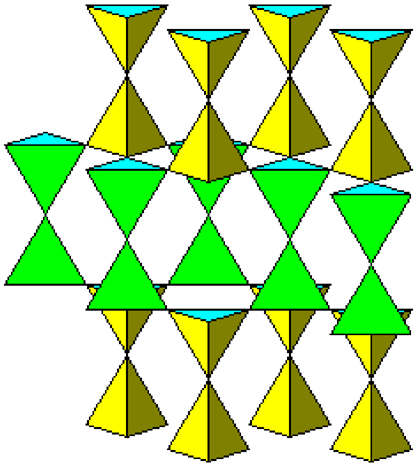


filosilicatos

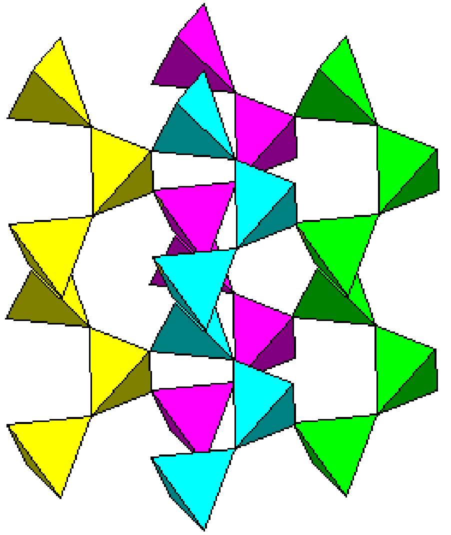


mica

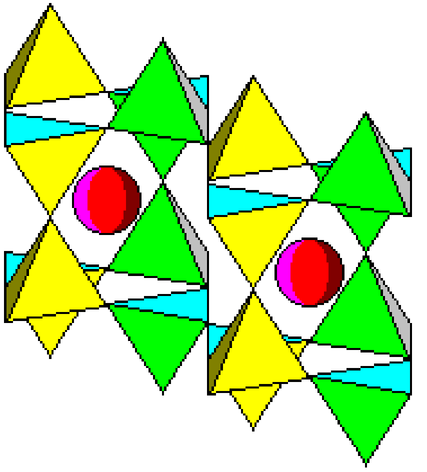
Armazones estructurales tectosilicatos



Tridimita (SiO_2)



Cuarzo (SiO_2)

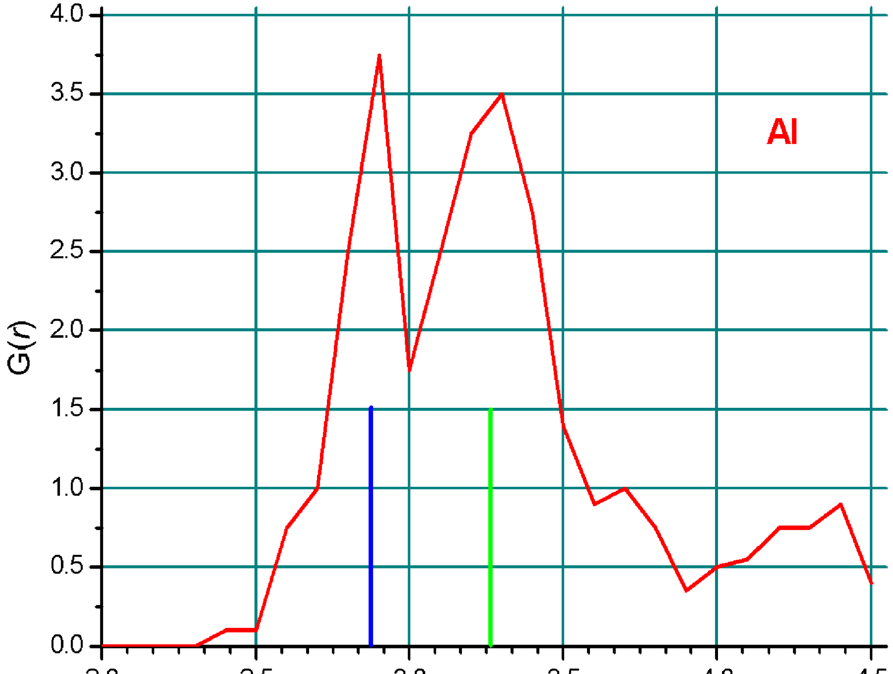


Feldespatos

Un modelo cristaloquímico alternativo

Material cedido por el profesor Ángel Vegas

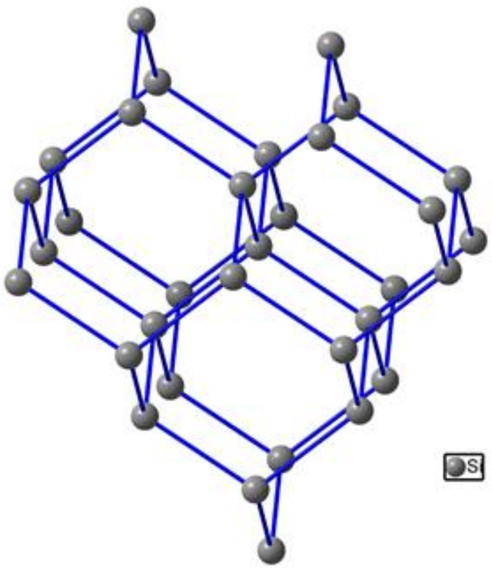
Los óxidos mantienen la topología y las distancias del metal del que provienene



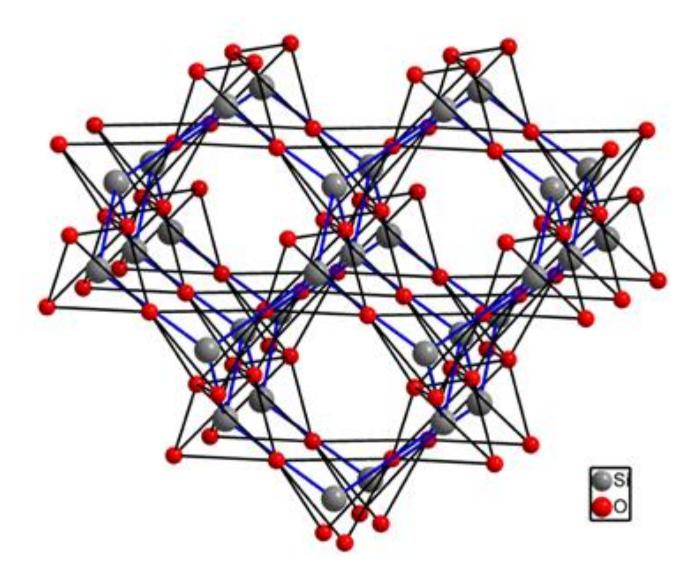
***fcc*-Al, a = 4.04 Å**

$d_{Al\text{-}Al}$ = 2.86 Å

Alrededor de 2700 compuestos

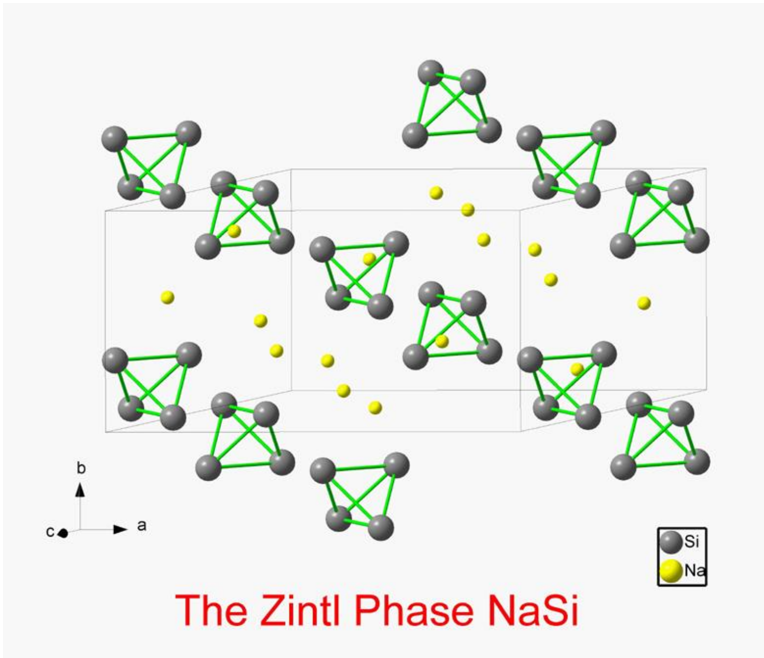


Si

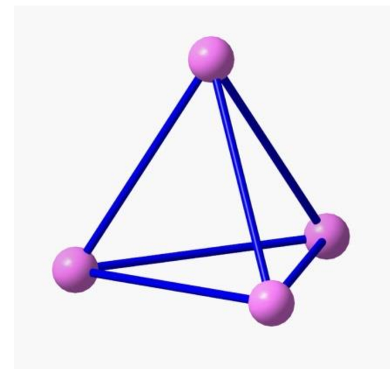


SiO_2- Cristobalite

El concepto de Zintl-Klemm: Fases de Zintl



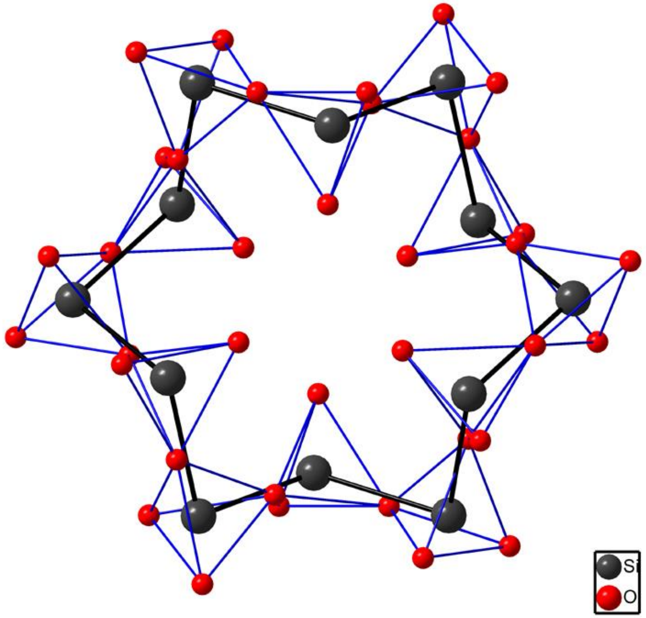
NaSi: Si as Ψ-P $(Si_4)^{4-}$

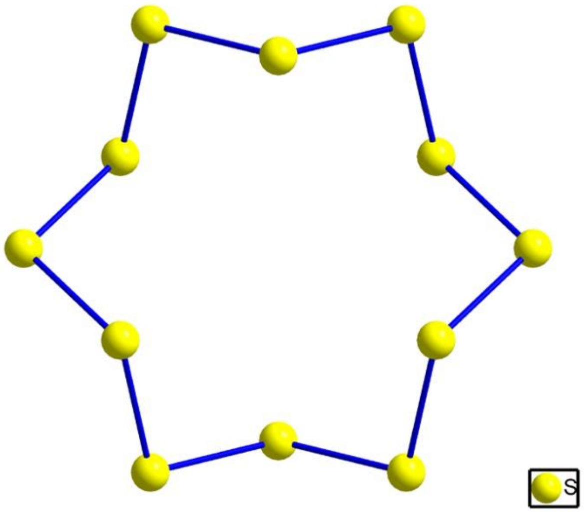


The P_4 molecule

Aplicación del concepto de Zintl-Klemm a las estructuras de los silicatos

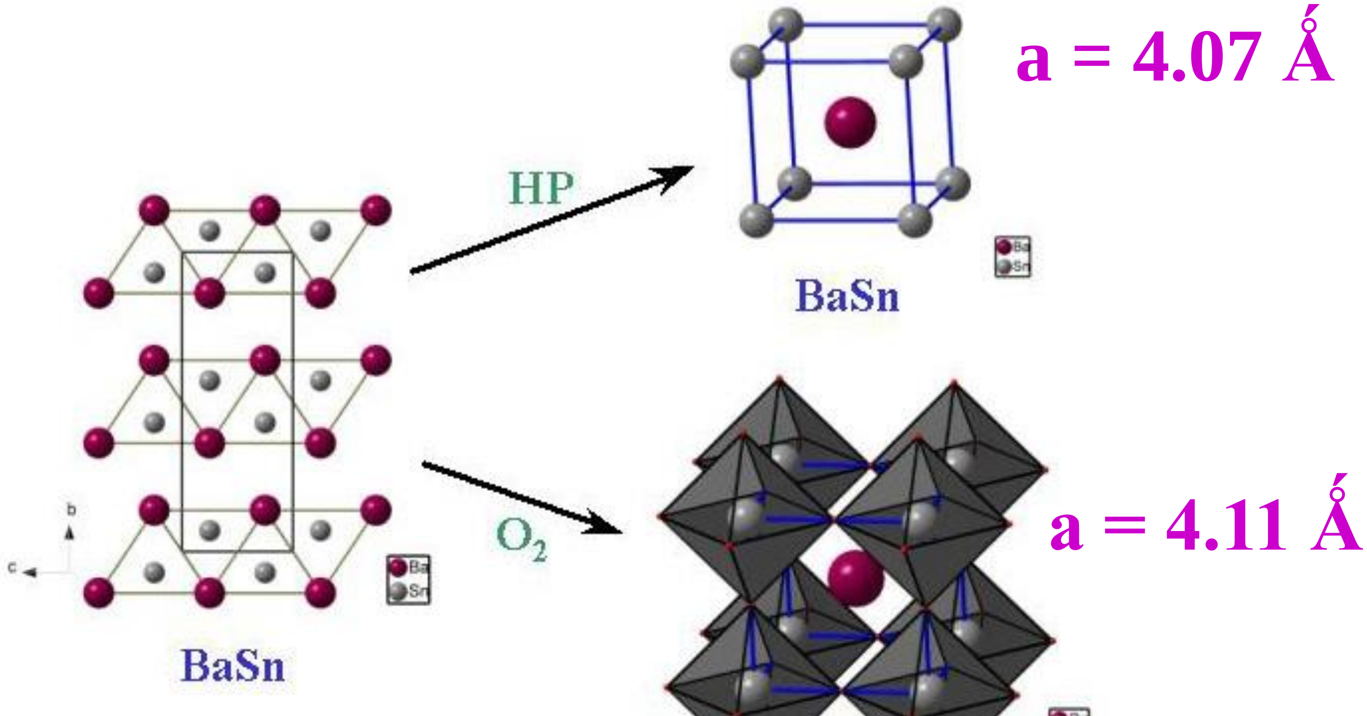
Ejemplo: ciclosilicatos





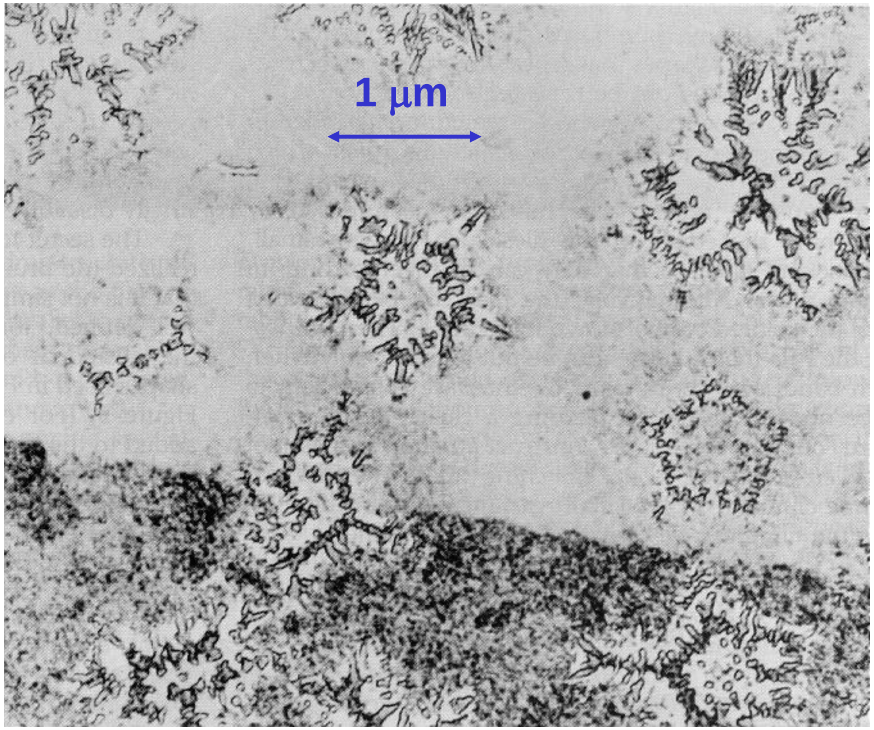
Equivalencia entre oxidación y presión

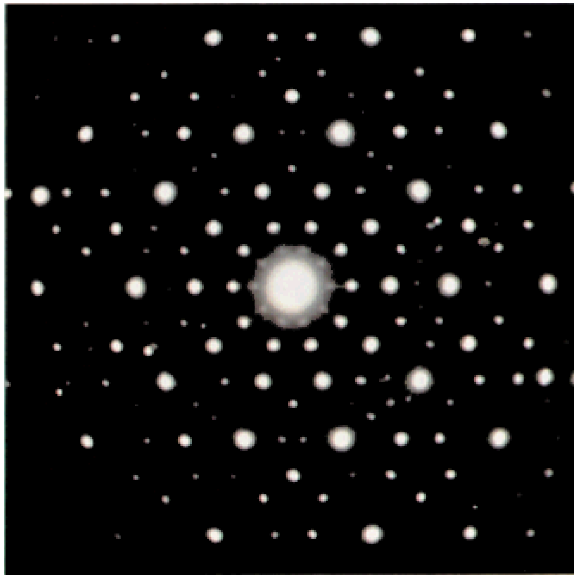
Beck & Lederer, 1993 → Vegas et al. 1994



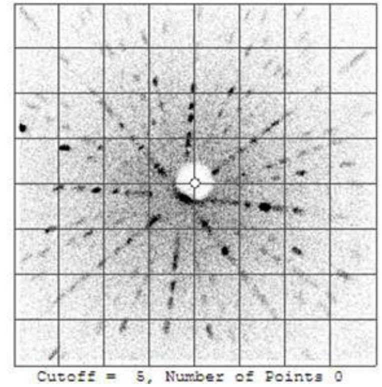
CUASICRISTALES

Al_6Mn

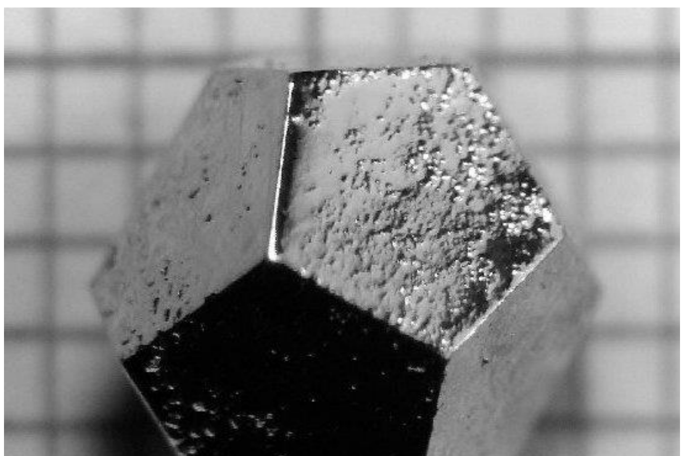


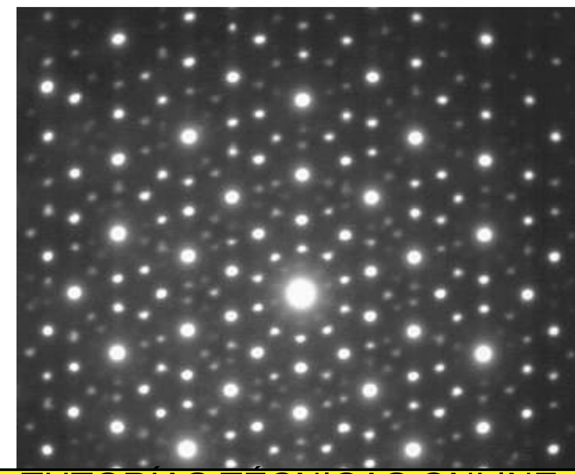


Pirita (FeS_2)



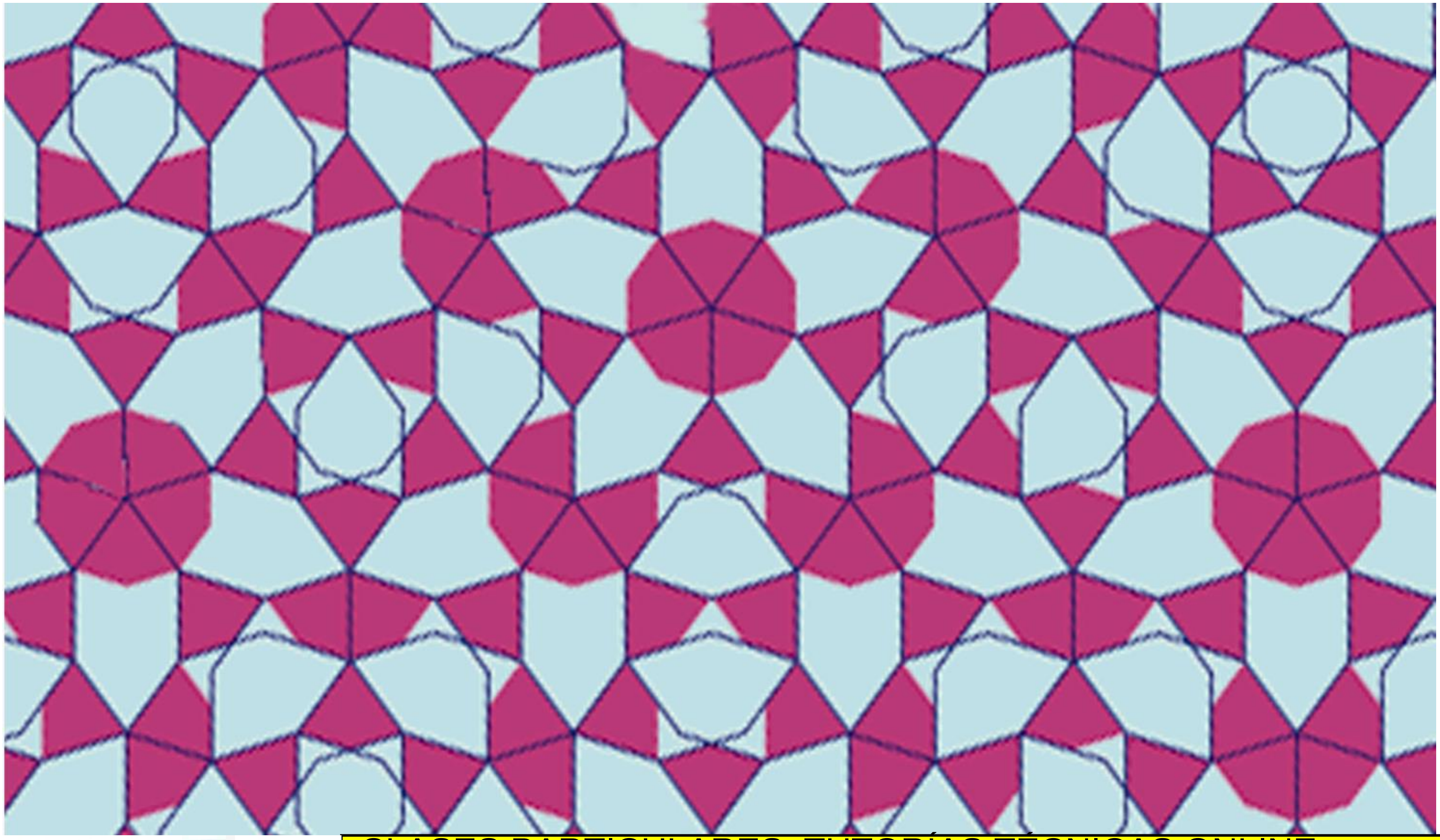
Patrón de difracción de un cristal de pirita

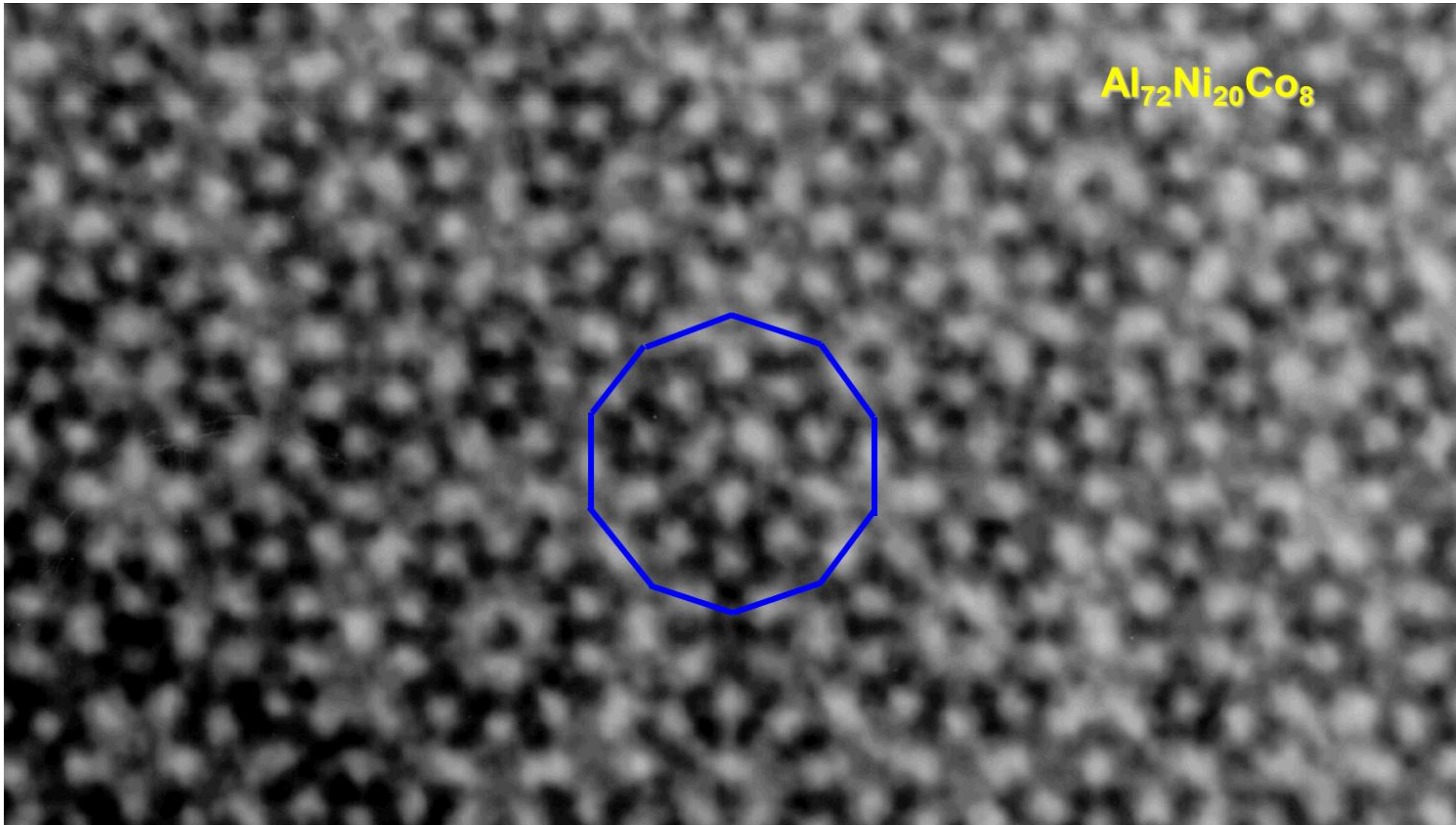




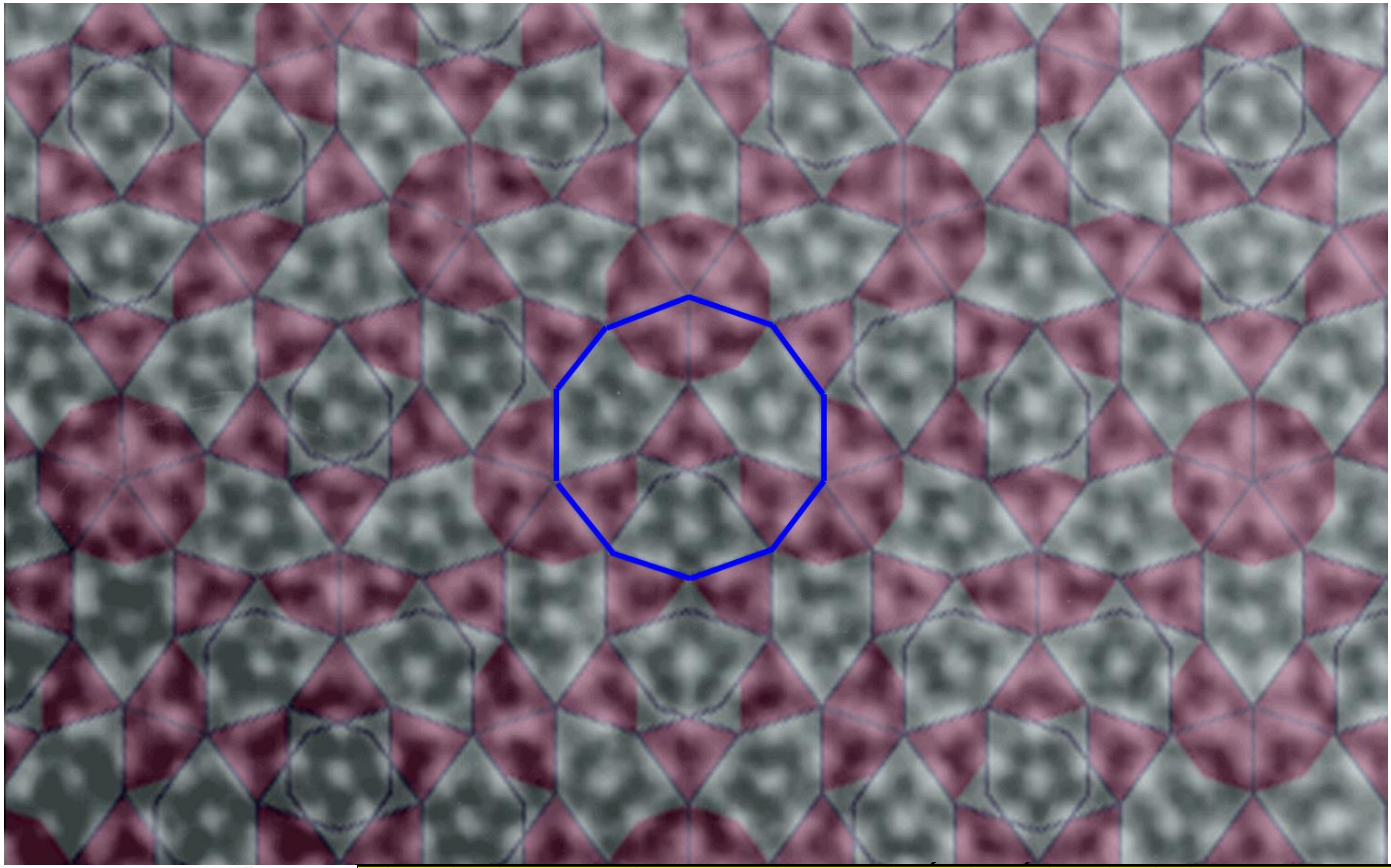
¡ Los cuasicristales no cumplen la condición $\boldsymbol{2\cos\alpha = Z}$!

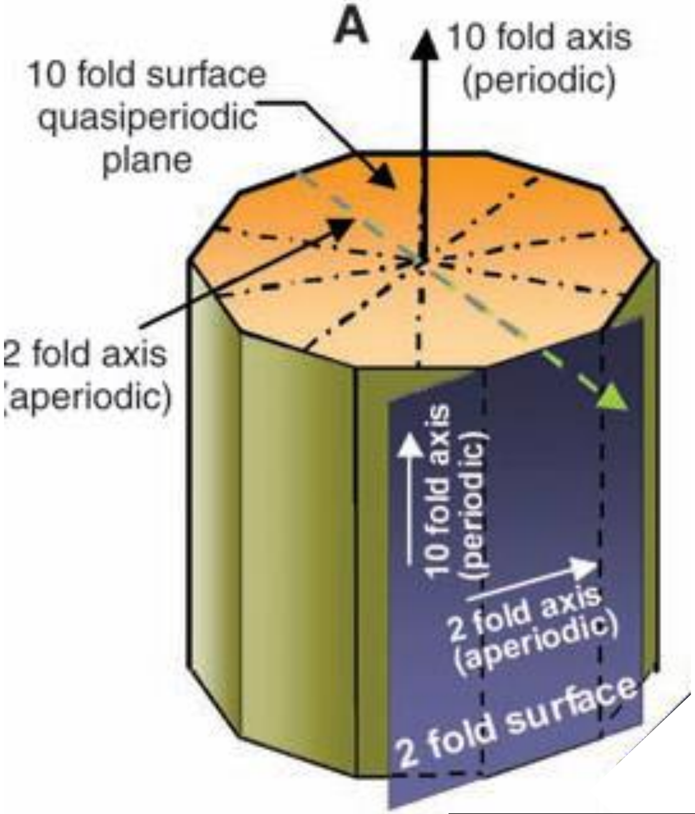
TESELADOS DE PENROSE

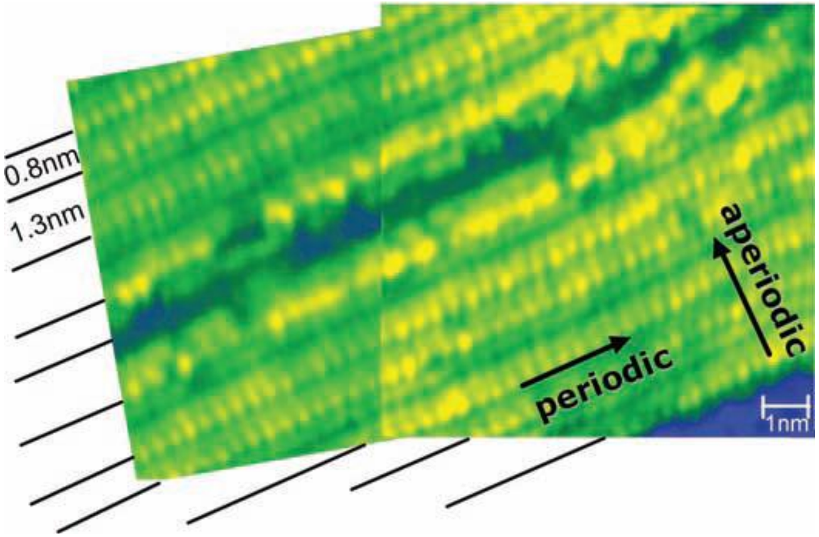




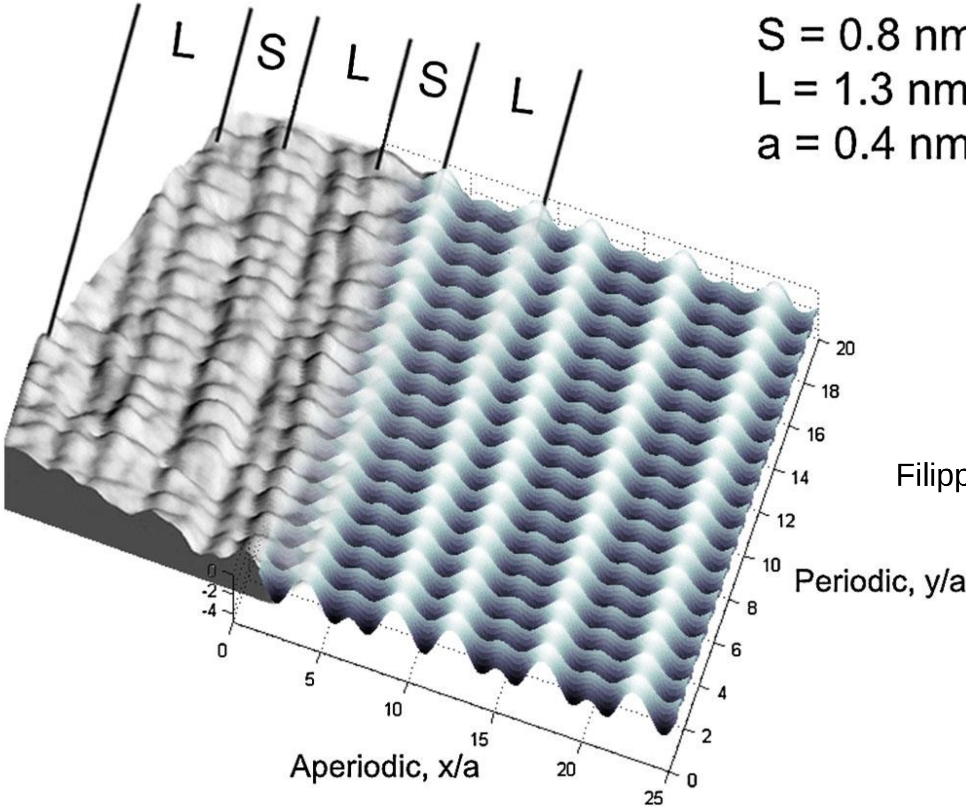
Nature 396, 55-57 (1998)







Park et al, Science 2005



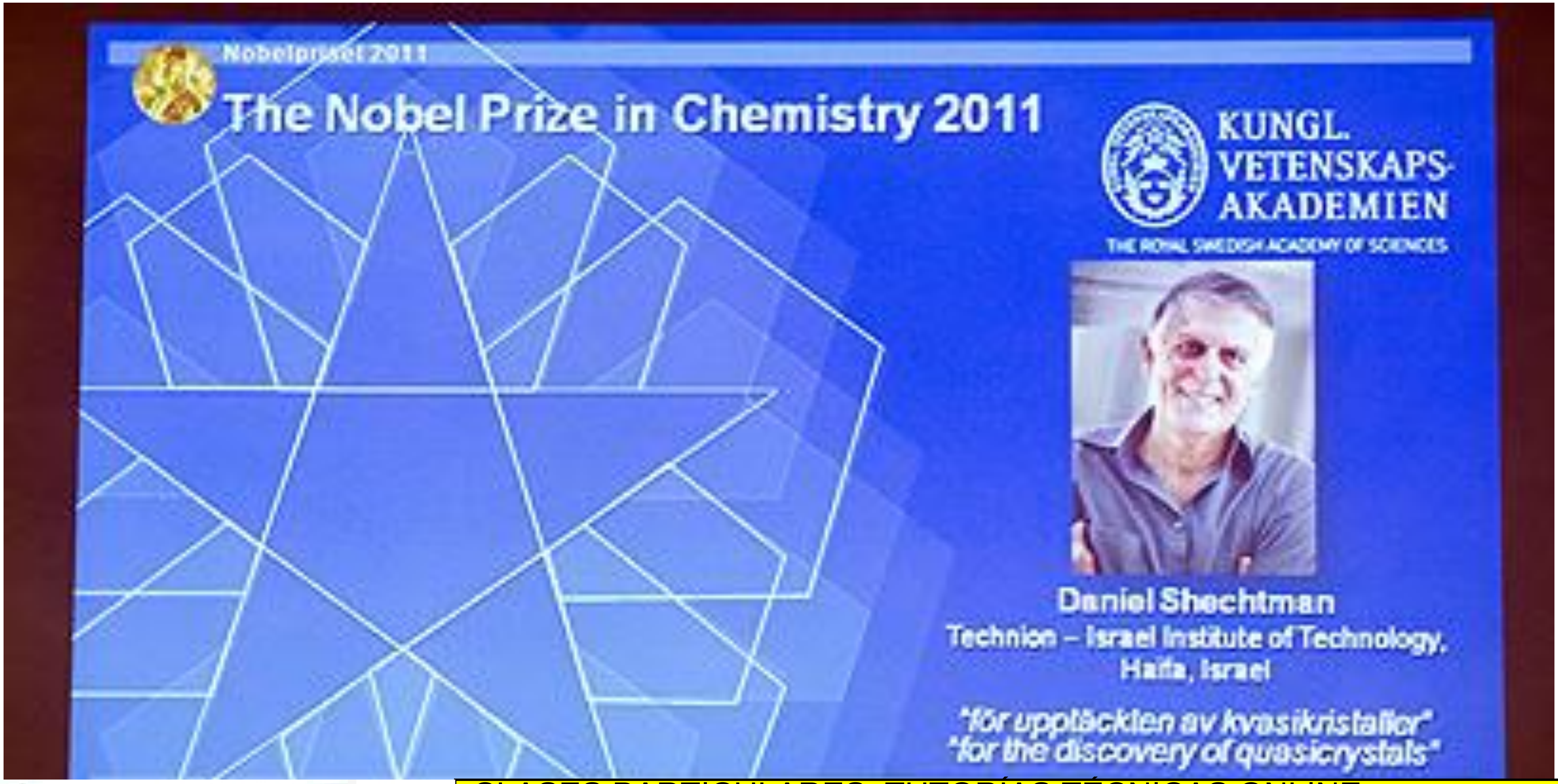
S = 0.8 nm
L = 1.3 nm
a = 0.4 nm

Filippov et al PRL 2010

SLLSLLSLSLLSLLSLSLLSLSL

Secuencia de Fibonacci

S
L
LS


Nobelpriset 2011
The Nobel Prize in Chemistry 2011
KUNGL. VETENSKAPS-AKADEMIEN
THE ROYAL SWEDISH ACADEMY OF SCIENCES
Daniel Shechtman
Technion – Israel Institute of Technology, Haifa, Israel
"för upptäckten av kvasikristaller"
"for the discovery of quasicrystals"

A commercial application: