Crystal structures

CIF files and programs to visualize crystal structures

Crystal structure data is often stored in a CIF file. This is a text file that contains the asymmetric unit of the crystal, the symmetries of the space group, and a reference to the source where the data was first published. It is important to check the publication to see the conditions used during the experiment. Some experiments are performed at high temperatures or high pressures where the crystal structure can be different than at room temperature and ambient pressure. The links below will display a crystal structure and it's corresponding CIF file.

Simple Cubic, Polonium Po $Pm\bar{3}m$ #221
Face-centered Cubic (fcc) $Fm\bar{3}m$ #225
Body-centered Cubic (bcc) $Im\bar{3}m$ #229
Hexagonal, Boron nitride BN #194
Hexagonal Close Packed (hcp) P63/mmc #194
Perovskite, Calcium titanate $CaTiO_3$ (perovskite) $Pm\bar{3}m$ #221
Caesium chloride CsCl $Pm\bar{3}m$ #221
Rocksalt NaCl $Fm\bar{3}m$ #225
Zincblende #216
Wurtzite #186
Diamond (C) #227
β-Sn #141
Graphite C P63mc #186

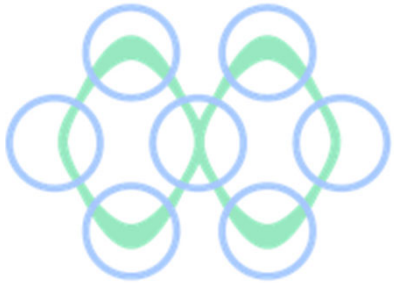
Sucrose P21 #4
Magnetite Fe_3O_4 Fd3m #227
Cementite Fe_3C #62
Copper oxide CO (Tenorite) #15
Pyrite FeS_2 #205
Rutile TiO_2 #136
Spinel $MgAl_2O_4$ #227
$Sr_2FeMoO6_6$ (double perovskite) I4/mmm #139
$YBa_2Cu_3O_7$ #47
ZIF8 #1
Zinc oxide ZnO (wurtzite) P63mc #186
ZnS (wurtzite) #186

Prototypes | Periodic Table | Semiconductors | Ceramics

Encyclopedia of Crystallographic Prototypes

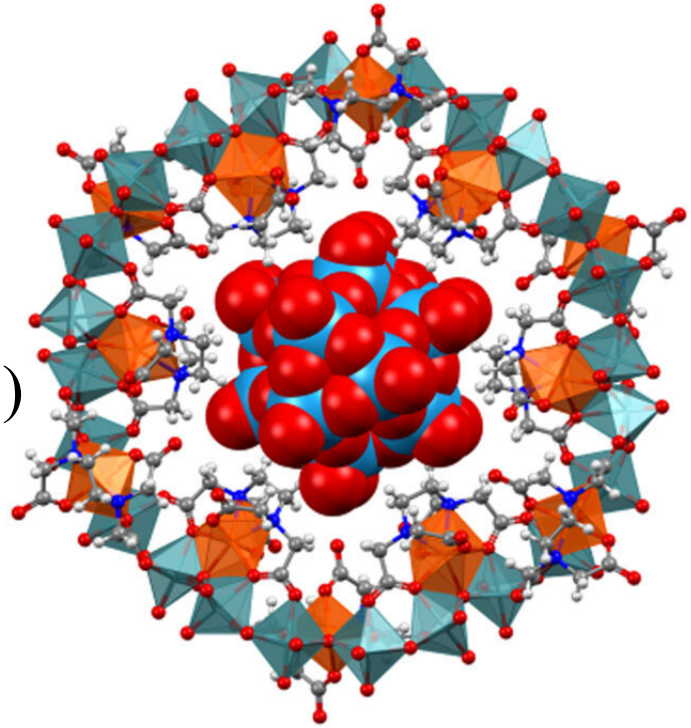
ICSD

Inorganic Crystal Structure Database

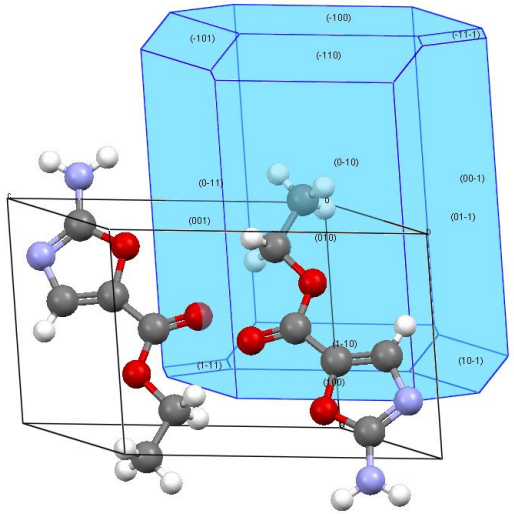


Materials Project

Free Mercury



Cambridge Structural Database (CSD)



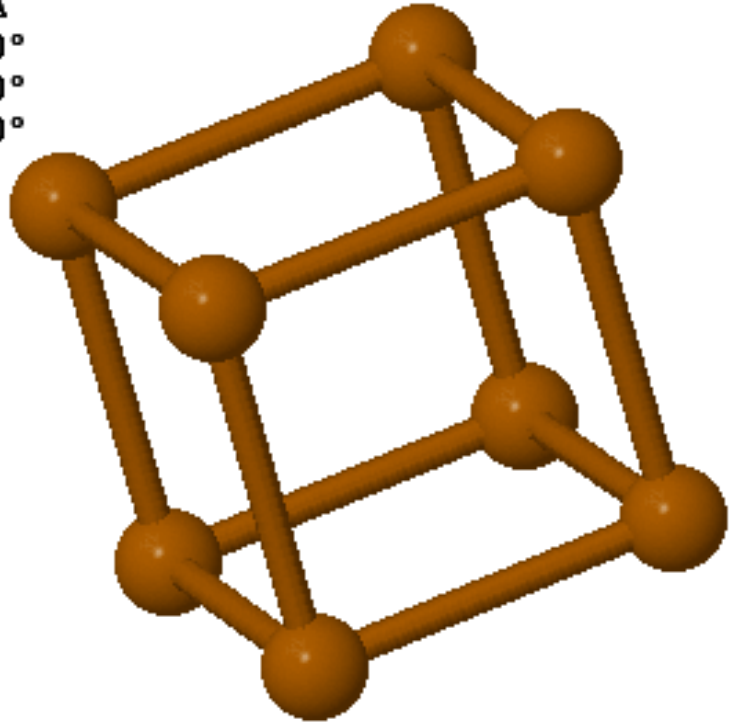
Standard data file: *.cif

https://www.ccdc.cam.ac.uk/Community/csd-community/freemercury/

simple cubic

Po

HM:P m -3 m
a=3.359Å
b=3.359Å
c=3.359Å
α=90.000°
β=90.000°
γ=90.000°



Number: 221

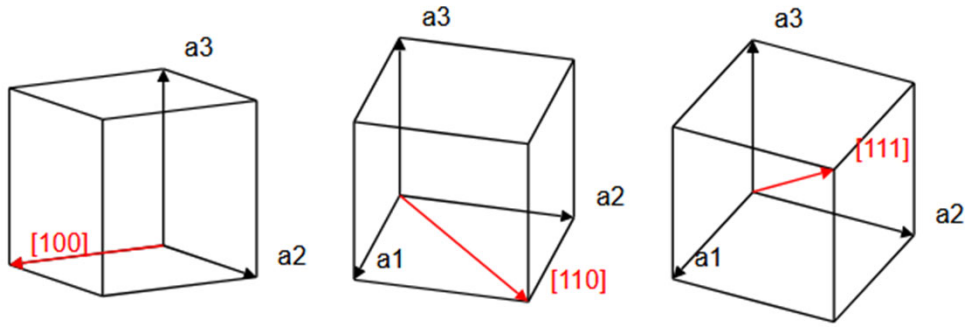
Primitive Vectors:

$$\vec{a}_1 = a\hat{x}$$

$$\vec{a}_2 = a\hat{y}$$

$$\vec{a}_3 = a\hat{z}$$

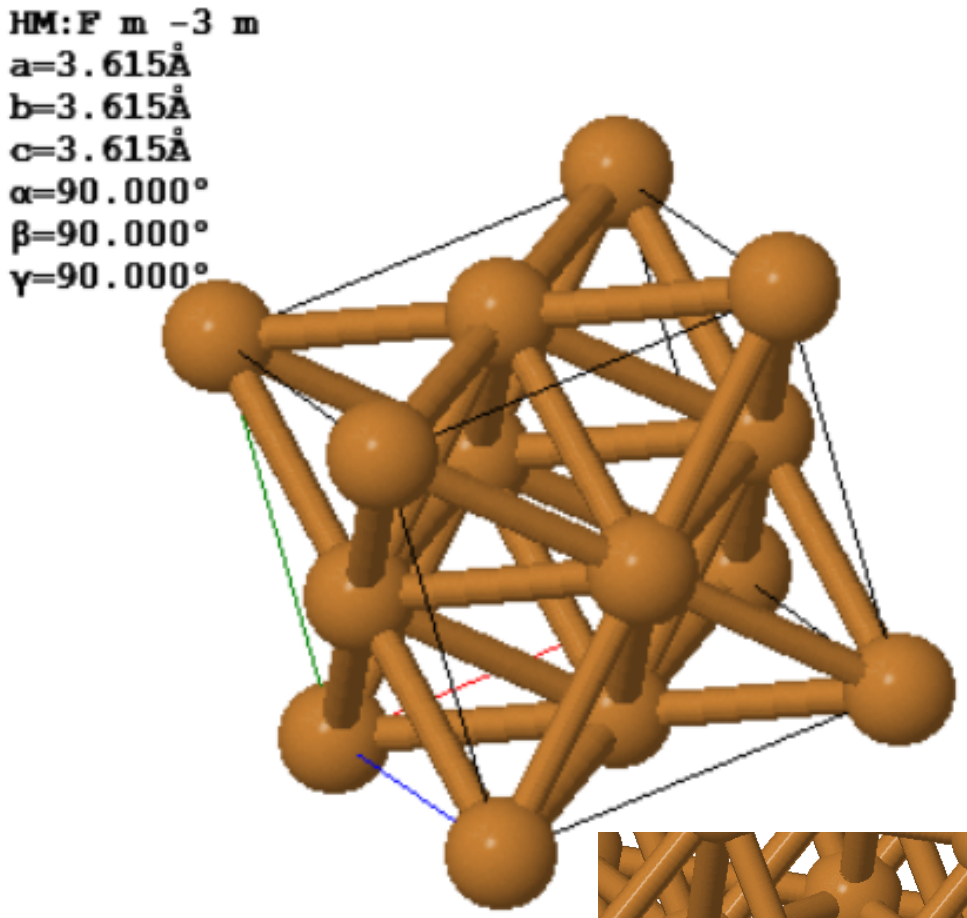
Basis Vector: $\vec{B}_1 = (0,0,0)$



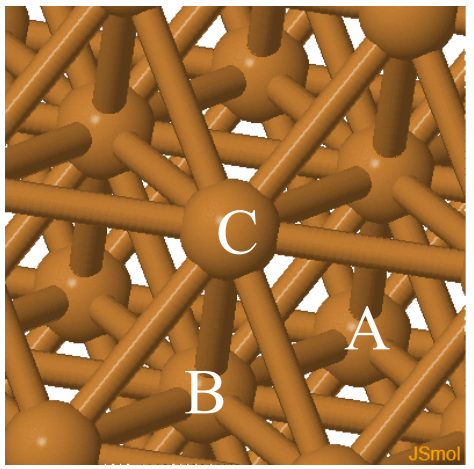
fcc

Number 225

Al, Cu,
Ni, Sr,
Rh, Pd,
Ag, Ce,
Tb, Ir,
Pt, Au,
Pb, Th



[111]



Primitive Vectors:

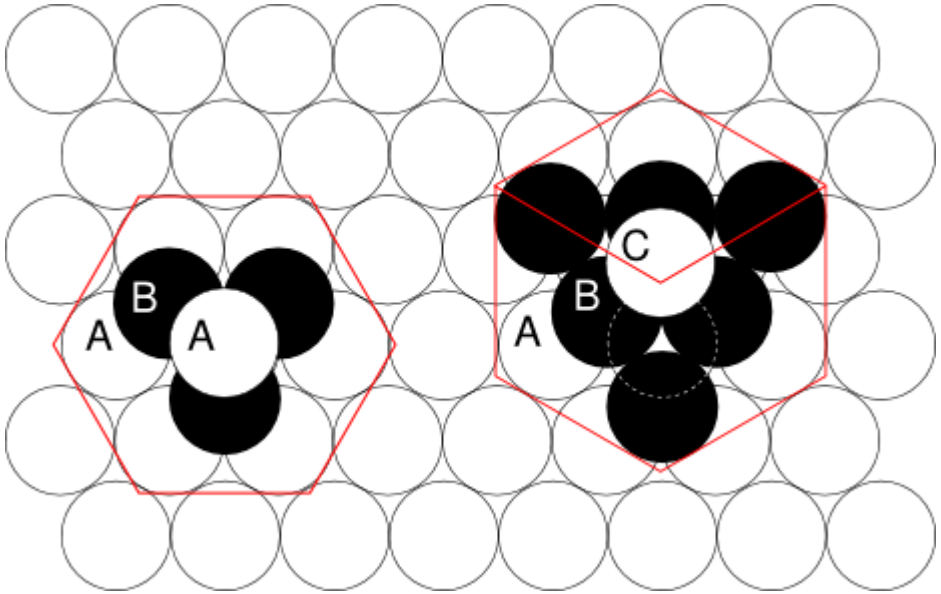
$$\vec{a}_1 = \frac{a}{2}\hat{y} + \frac{a}{2}\hat{z}$$

$$\vec{a}_2 = \frac{a}{2}\hat{x} + \frac{a}{2}\hat{z}$$

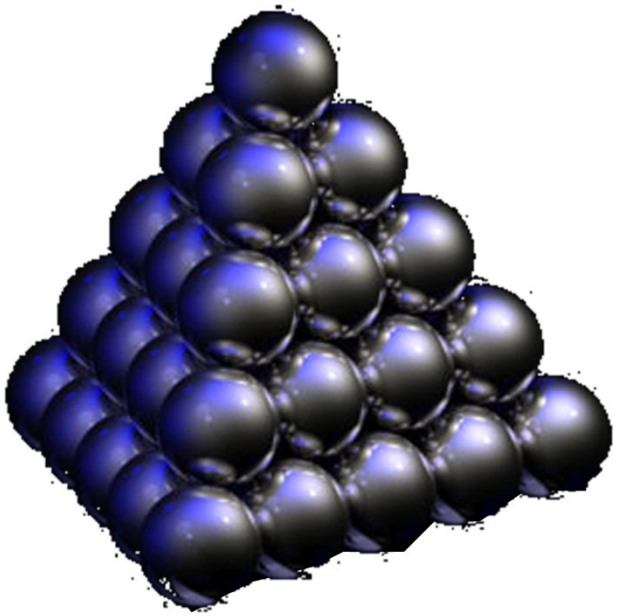
$$\vec{a}_3 = \frac{a}{2}\hat{x} + \frac{a}{2}\hat{y}$$

Basis Vector: $\vec{B}_1 = (0,0,0)$

Close packing



HCP FCC

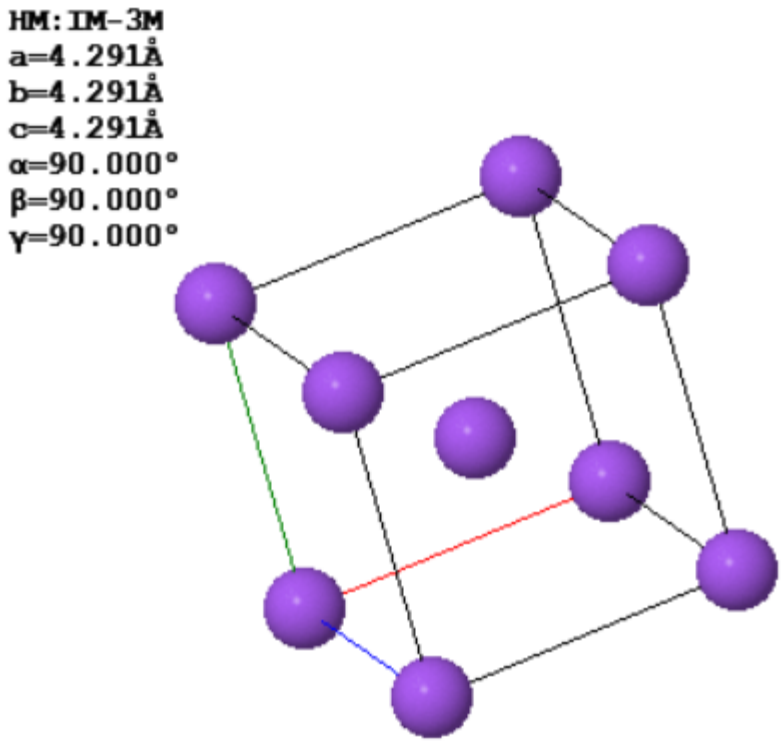


HCP = Hexagonal close pack
Hexagonal Bravais lattice with two atoms in the basis.

bcc

W
Na
K
V
Cr
Fe
Rb
Nb
Mo
Cs
Ba
Eu
Ta

Number 229



Primitive Vectors:

$$\vec{a}_1 = -\frac{a}{2}\hat{x} + \frac{a}{2}\hat{y} + \frac{a}{2}\hat{z}$$

$$\vec{a}_2 = \frac{a}{2}\hat{x} - \frac{a}{2}\hat{y} + \frac{a}{2}\hat{z}$$

$$\vec{a}_3 = \frac{a}{2}\hat{x} + \frac{a}{2}\hat{y} - \frac{a}{2}\hat{z}$$

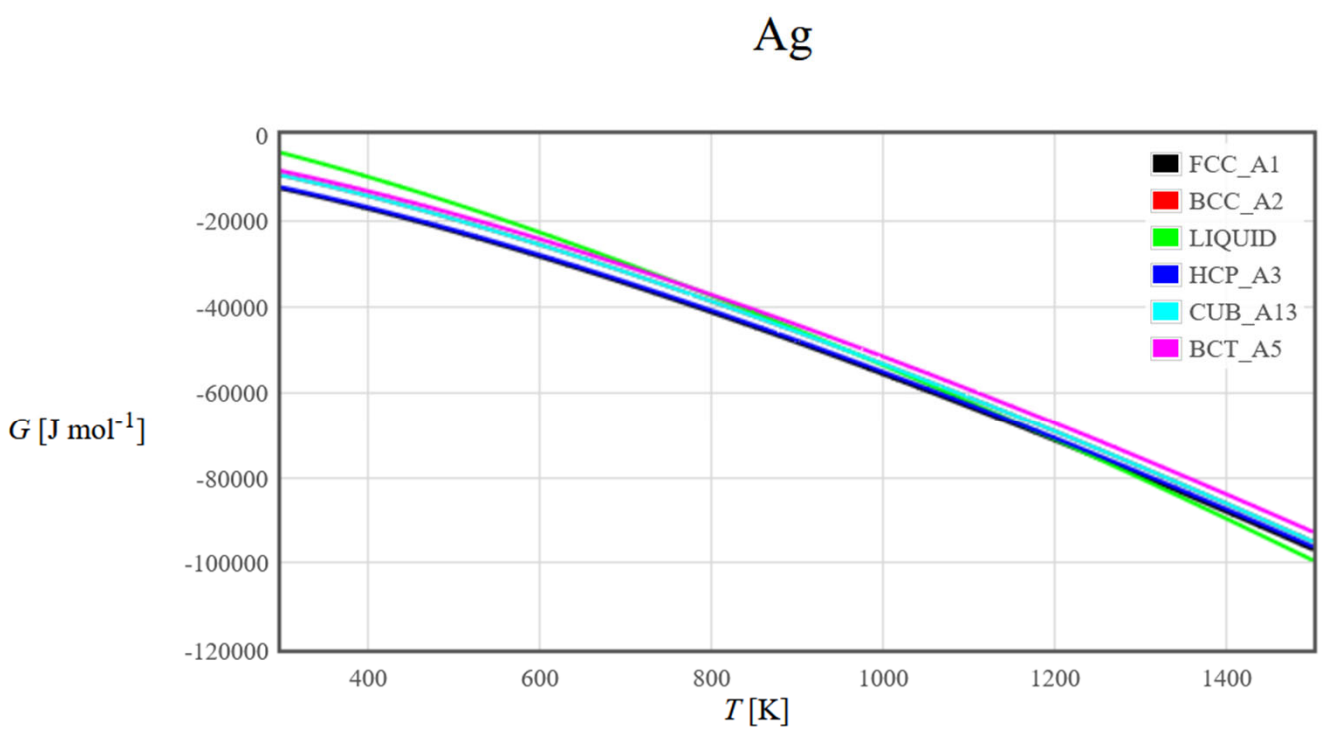
Basis Vector: $\vec{B}_1 = (0,0,0)$

SGTE thermodynamic data

The Scientific Group Thermodata Europe SGTE maintains thermodynamic databanks for inorganic and metallurgical systems. Data from their 'pure element database' is plotted below.

Typically, experiments are performed at constant pressure p, temperature T, and number N. Under these conditions, the system will go to the minimum of the Gibbs energy $G = U + pV - TS$. Here U is the internal energy, V is the volume, and S is the entropy. The top plot is the Gibbs energy per mole.

Ag	Al	Am	As
Au	B	Ba	Be
Bi	C	Ca	Cd
Ce	Co	Cr	Cs
Cu	Dy	Er	Eu
Fe	Ga	Gd	Ge
Hf	Hg	Ho	In
Ir	K	La	Li
Lu	Mg	Mn	Mo
N	Na	Nb	Nd
Ni	Np	O	Os
P	Pa	Pb	Pd
Pr	Pt	Pu	Rb
Re	Rh	Ru	S
Sb	Sc	Se	Si
Sm	Sn	Sr	Ta
Tb	Tc	Te	Th
Ti	Tl	Tm	U

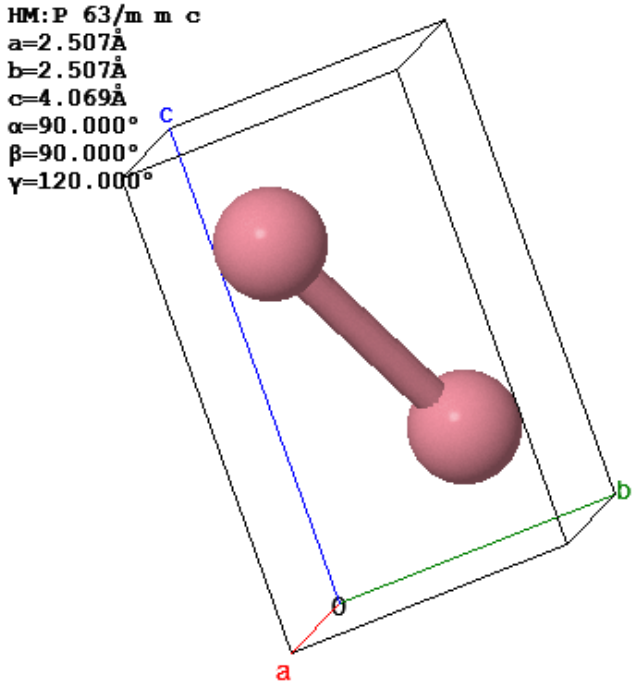


hcp

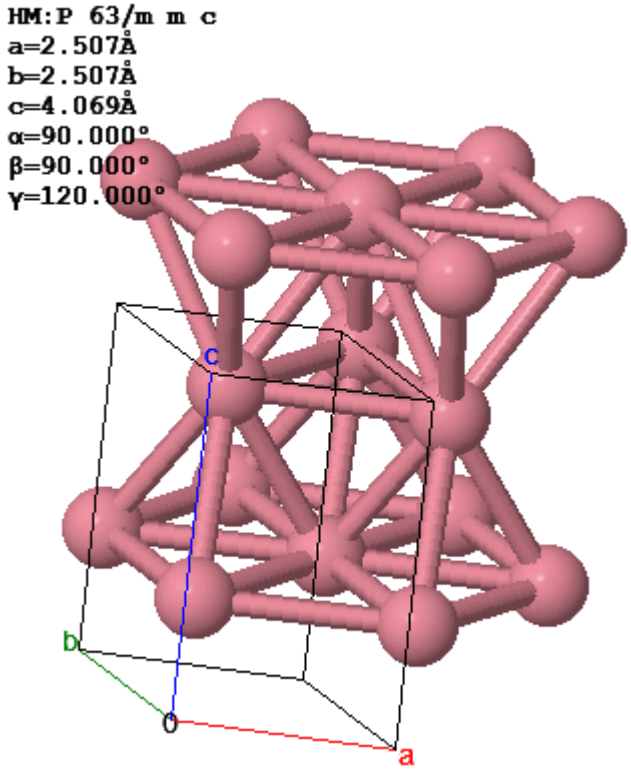
Space group 194

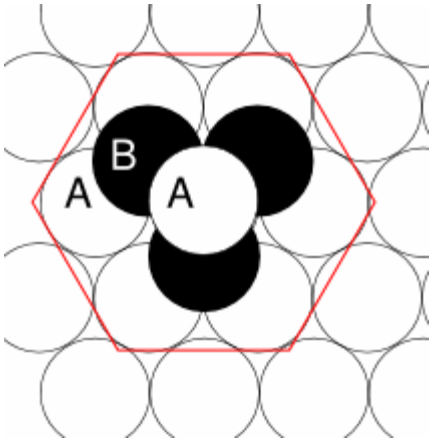
Mg, Be,
Sc, Ti,
Co, Zn,
Y, Zr, Tc,
Ru, Cd,
Gd, Tb,
Dy, Ho,
Er, Tm,
Lu, Hf,
Re, Os,
Tl

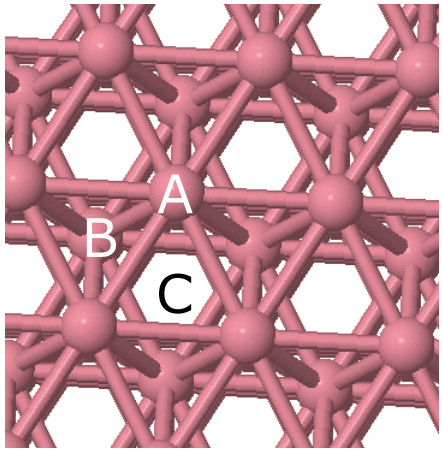
Crystallographic unit cell



Hexagonal unit cell



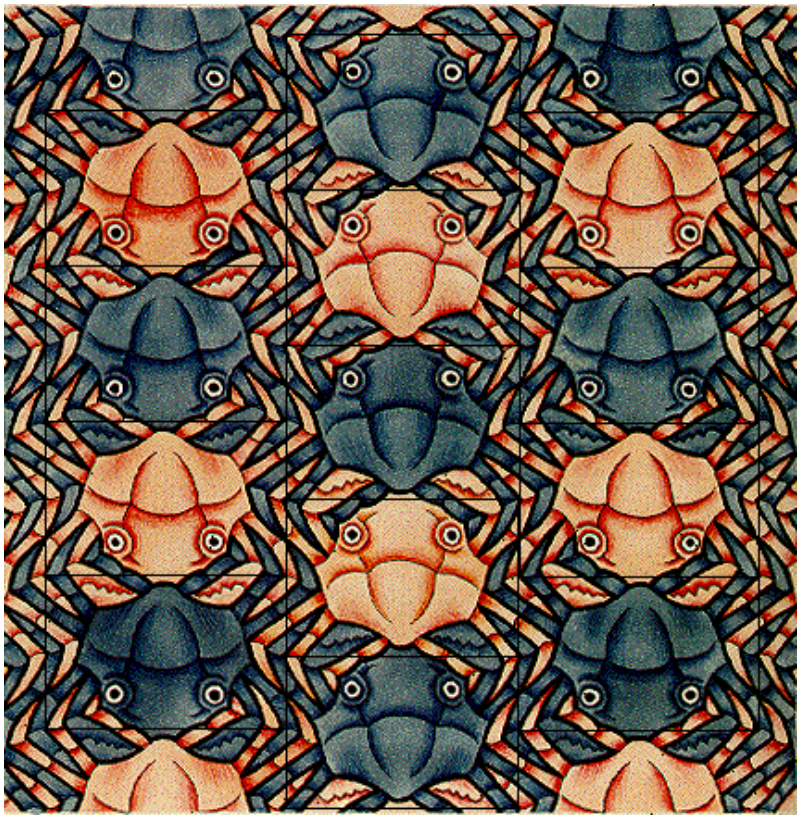




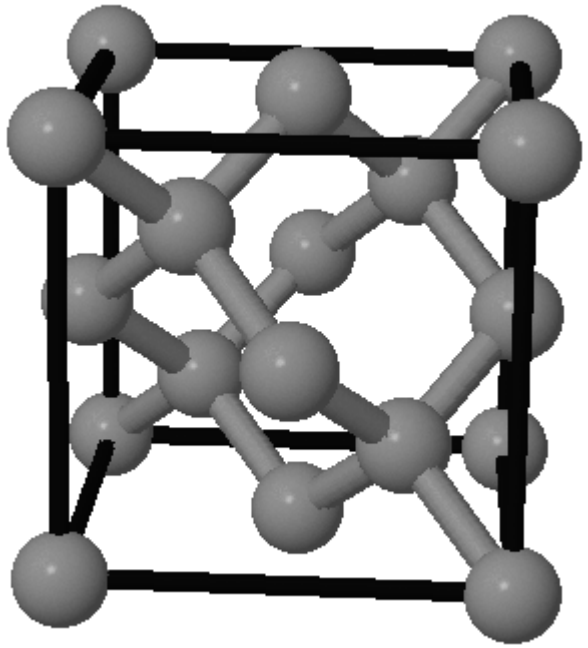
Hexagonal Bravais lattice
Basis vectors:

$$\vec{B}_1 = (0,0,0) \quad \vec{B}_2 = (\tfrac{2}{3},\tfrac{1}{3},\tfrac{1}{2})$$

Inequivalent atoms in the unit cell

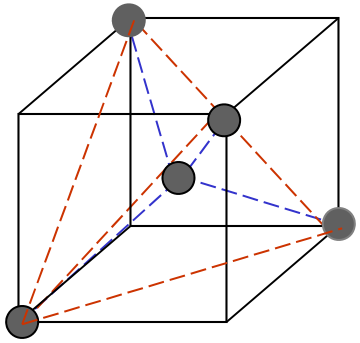


An element can have two distinct positions

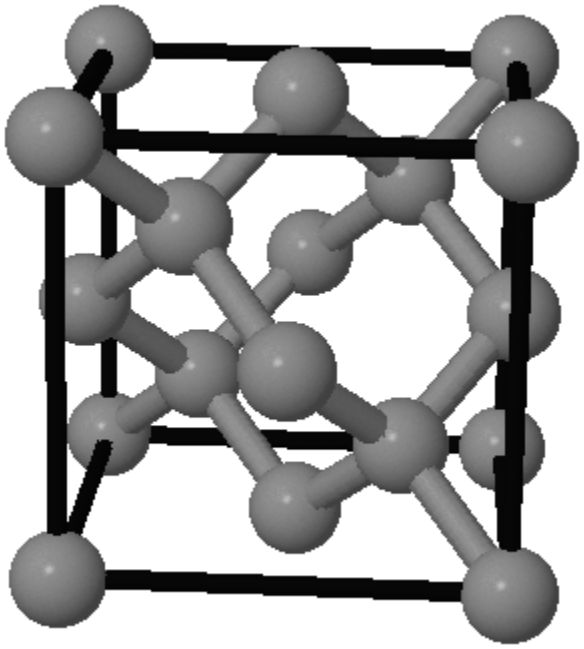


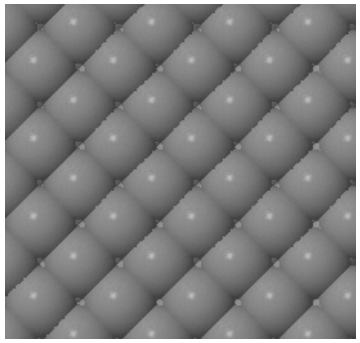
Diamond conventional unit cell

Diamond

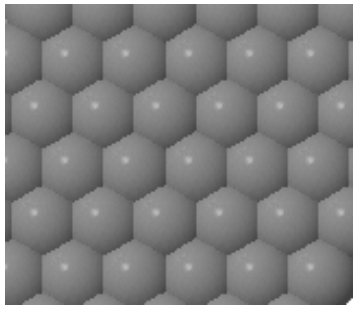


$$a = b = c, \quad \alpha = 90^\circ, \beta = 90^\circ, \gamma = 90^\circ$$





$$(100): \frac{2}{a^2}$$



$$(111): \frac{4}{\sqrt{3}a^2}$$

Space group: 227
point group: m3m

Primitive lattice vectors:

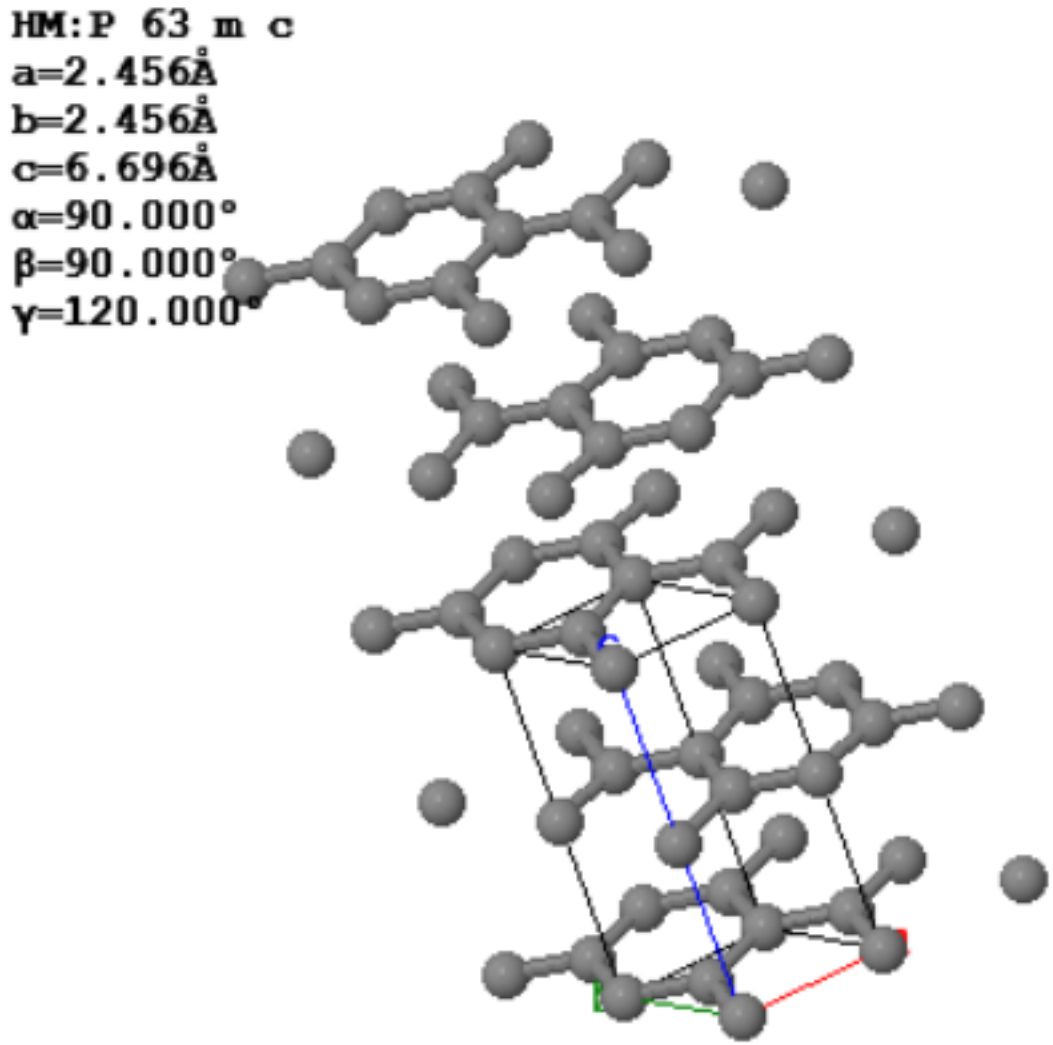
$$\vec{a}_1 = \frac{a}{2}\hat{x} + \frac{a}{2}\hat{y}, \qquad \vec{a}_2 = \frac{a}{2}\hat{x} + \frac{a}{2}\hat{z}, \qquad \vec{a}_3 = \frac{a}{2}\hat{y} + \frac{a}{2}\hat{z}.$$

Basis: $\vec{B}_1 = (0,0,0), \qquad \vec{B}_2 = (0.25, 0.25, 0.25).$

graphite

Space group 194

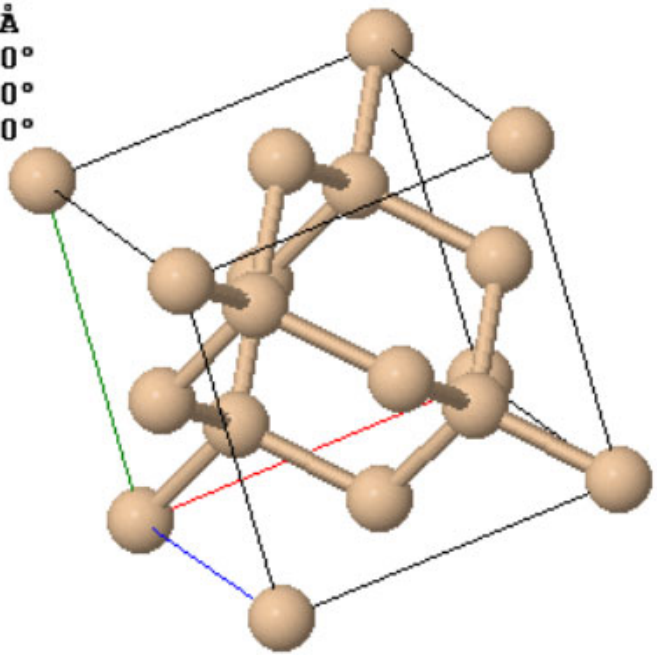
4 inequivalent C atoms in the primitive unit cell



Polytypes of carbon
graphite (hexagonal)
graphene
carbon nanotubes
diamond
rhobohedral graphite
hexagonal diamond

Silicon

HM:F d -3 m S
a=5.430Å
b=5.430Å
c=5.430Å
α=90.000°
β=90.000°
γ=90.000°



Conventional unit cell | Primitive unit cell | Asymmetric unit

2 x 2 x 2 | 3 x 3 x 3 | 5 x 5 x 5

Ball and Stick | Spacefill

H: 1 K: 0 L: 0

show HKL plane | hide HKL plane

draw atoms in HKL plane

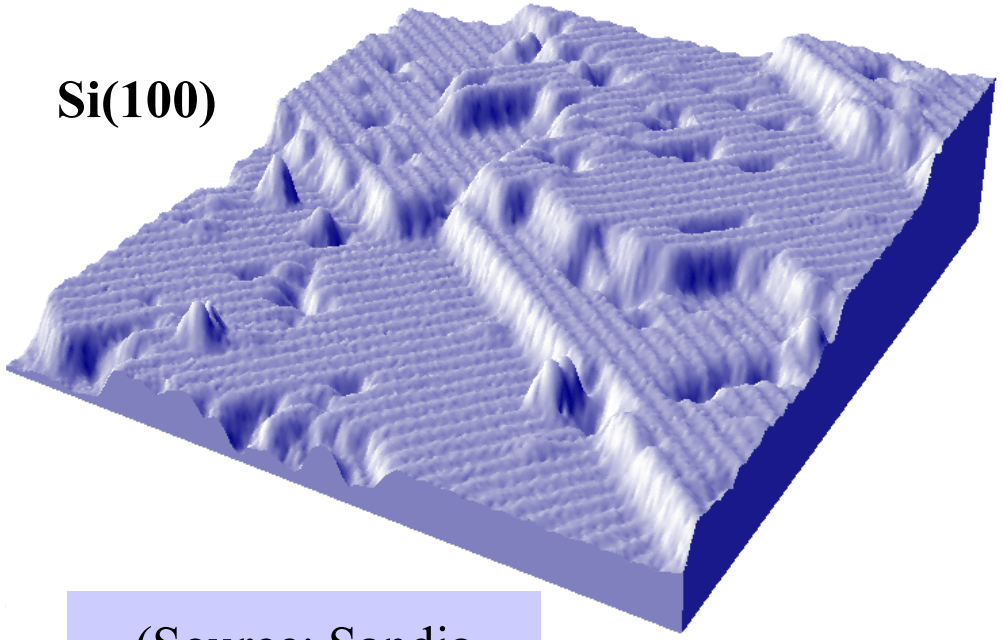
Thickness of HKL planes:

The conventional unit cell is a cube with sides of 0.543 nm. There are 8 atoms atoms in the conventional unit cell. (The image can be rotated with a mouse.)

JSmol

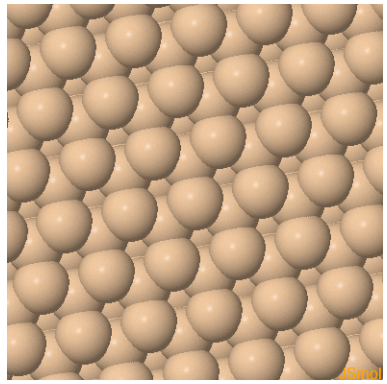
Silicon surfaces

Si(100)

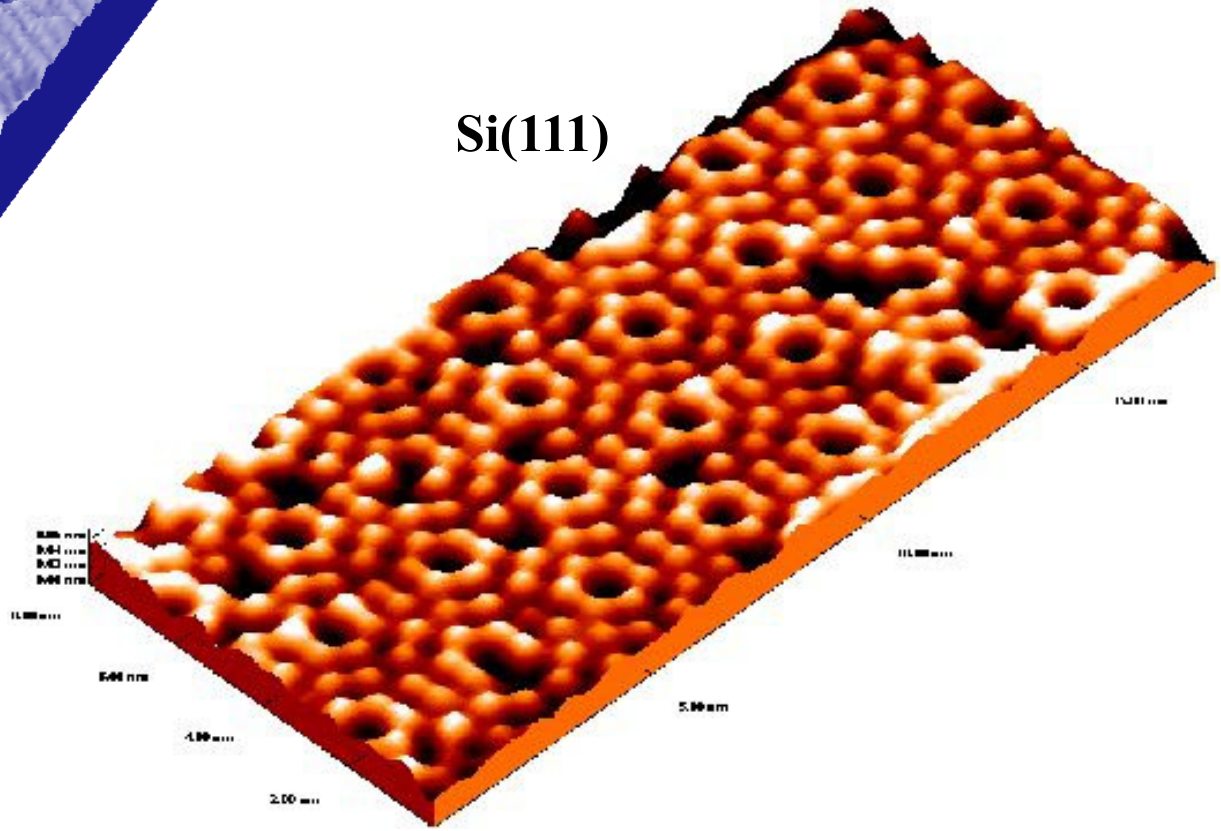


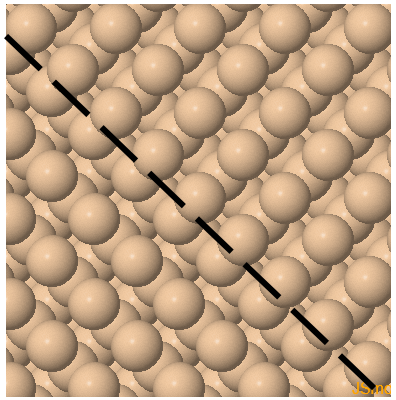
(Source: Sandia Nat.Labs.)

unreconstructed Si(111) →



Si(111)

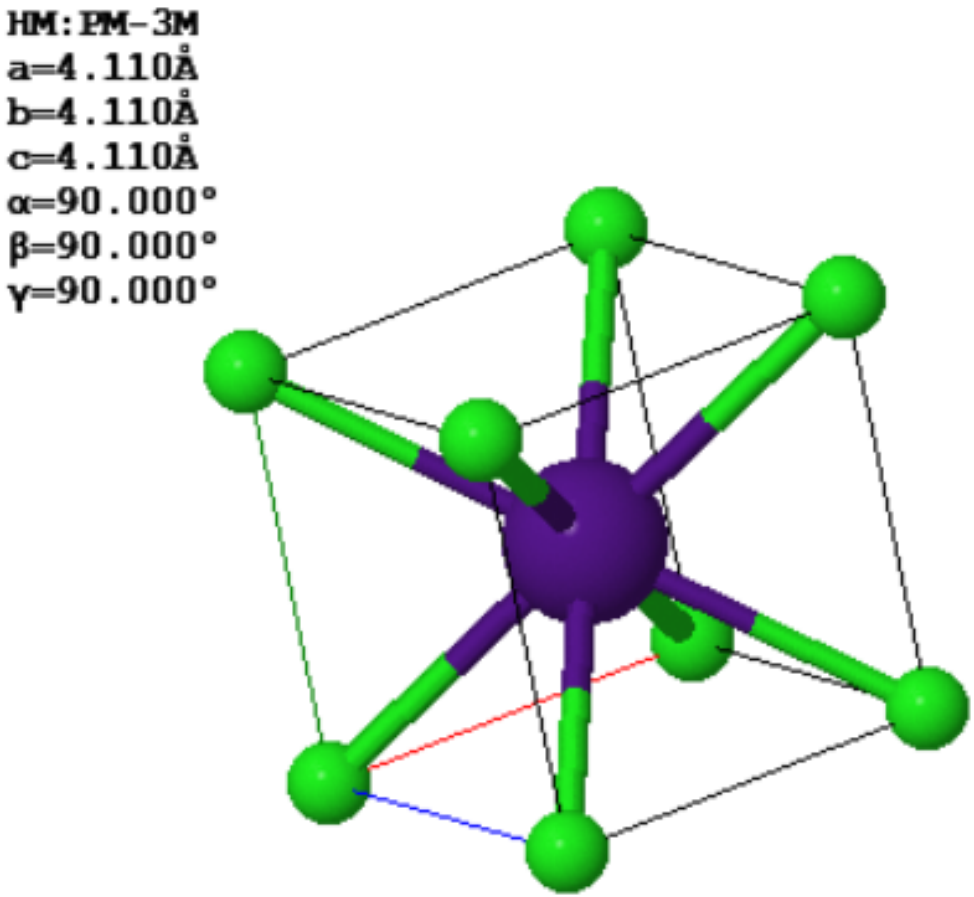




atomic step in Si(100)

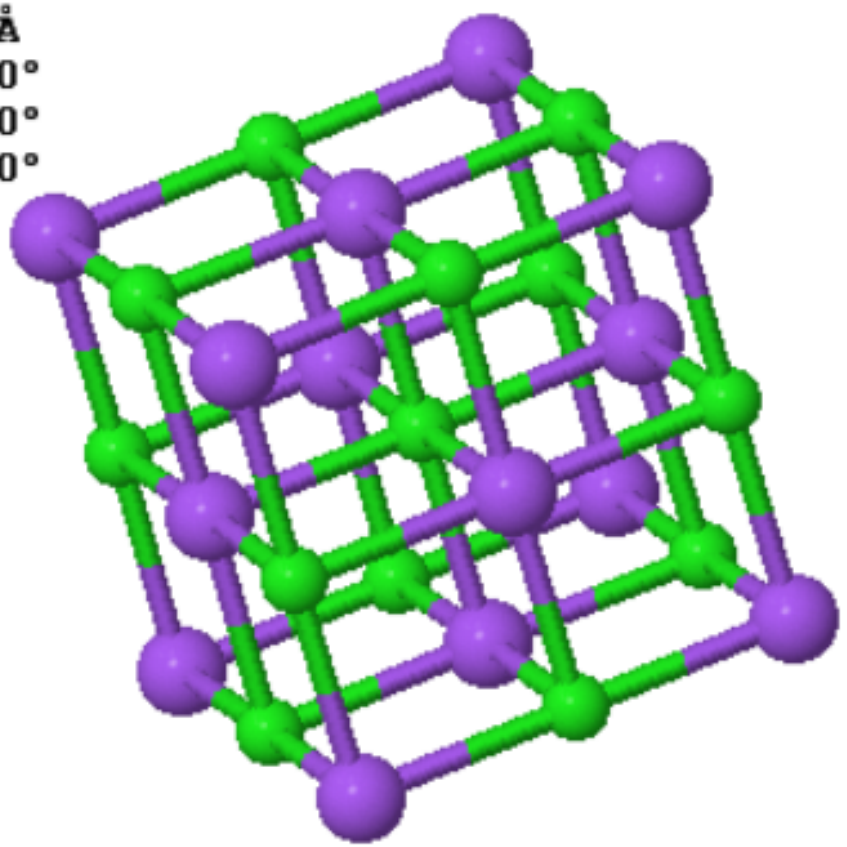
CsCl

Number 221



NaCl

HM:F m -3 m
a=5.639Å
b=5.639Å
c=5.639Å
α=90.000°
β=90.000°
γ=90.000°

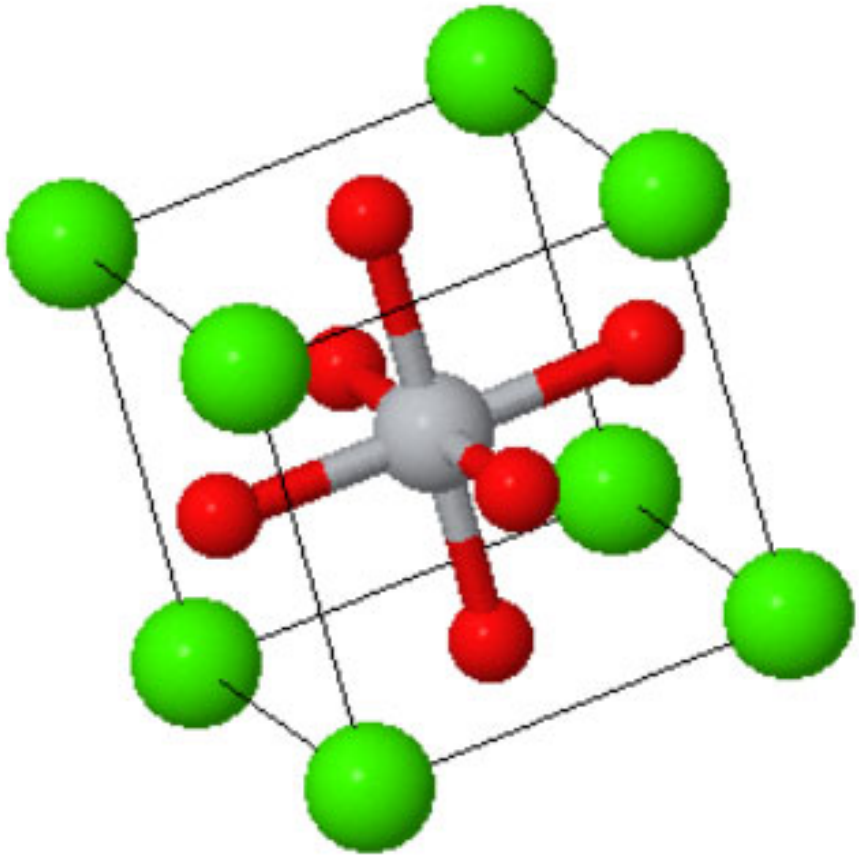


Number 225

perovskite

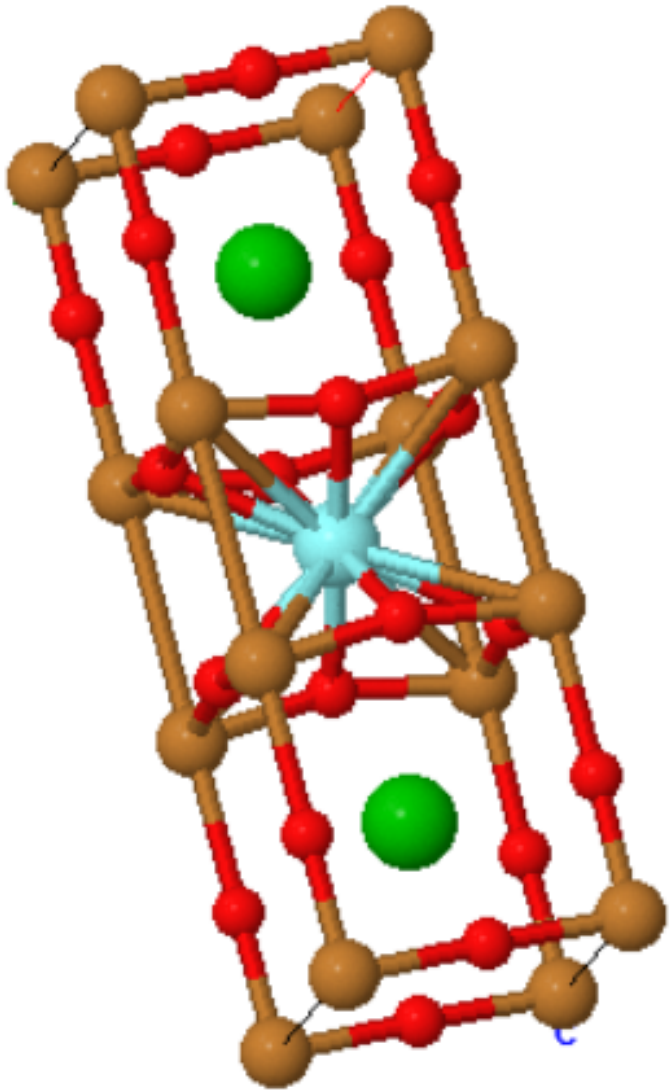
$SrTiO_3$
$LiNbO_3$
$BaTiO_3$
$Pb_xZr_{1-x}TiO_3$

Number 221



$YBa_2Cu_3O_7$

HM:P m m m
a=3.820Å
b=3.885Å
c=11.683Å
α=90.000°
β=90.000°
γ=90.000°

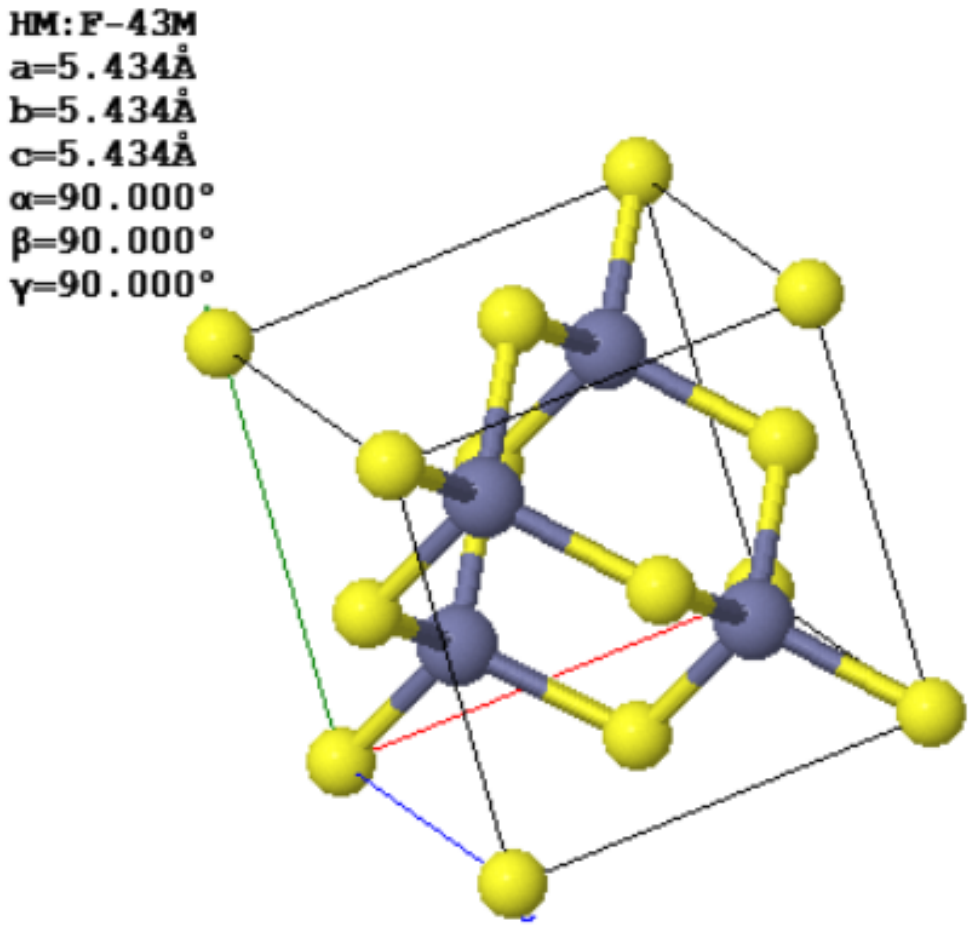


Number 47

zincblende

ZnS
GaAs
InP

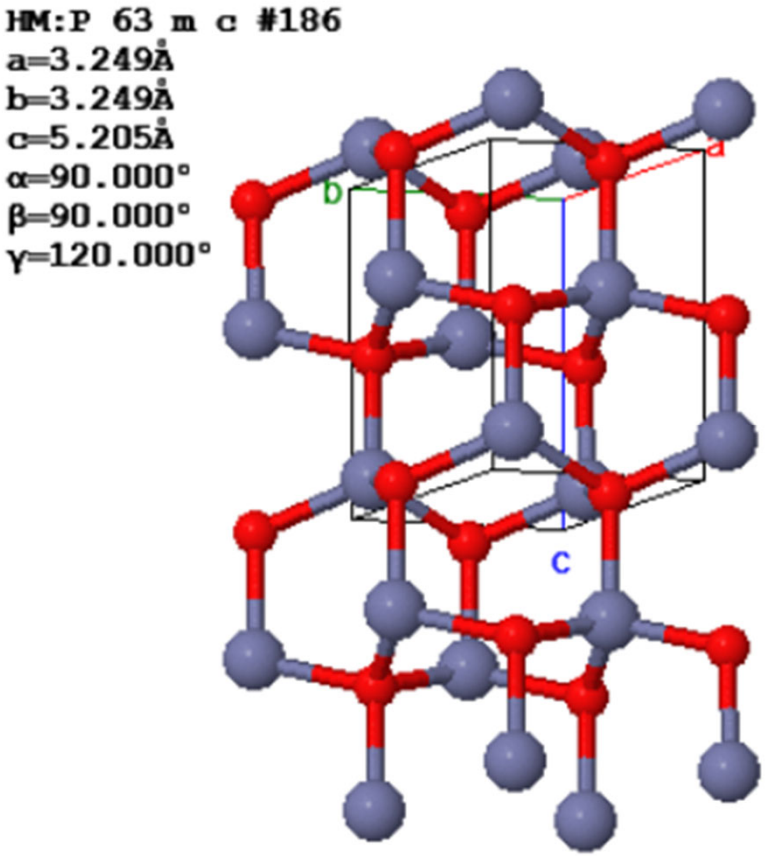
space group 216
$F\bar{4}3m$



wurtzite

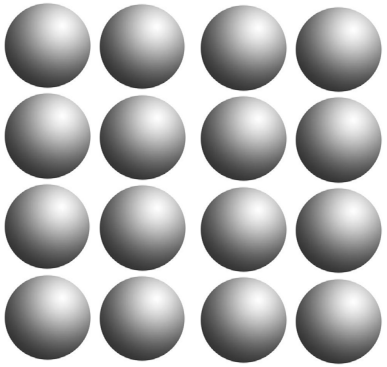
ZnS
ZnO
CdS
CdSe
GaN
AlN

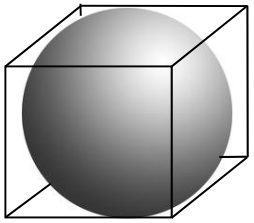
Number 186



There are 2 polytypes of ZnS: zincblende and wurtzite

atomic packing density



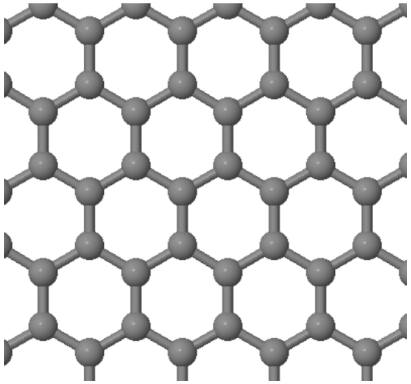


$$\frac{\frac{4}{3}\pi\left(L/2\right)^3}{L^3} = \frac{\pi}{6} \approx 0.52$$

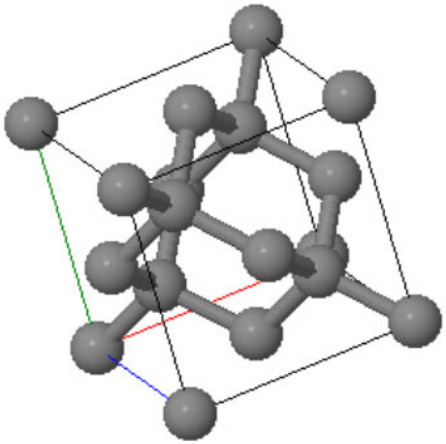
fcc, hcp = 0.74
random close pack = 0.64
simple cubic = 0.52
diamond = 0.34

Coordination number

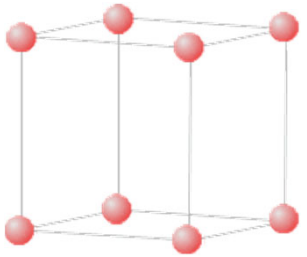
Number of nearest neighbors an atom has in a crystal



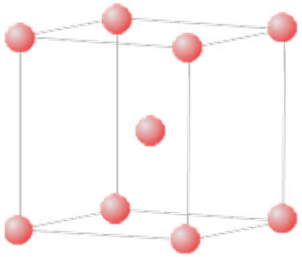
Graphene 3



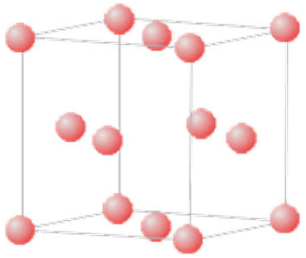
diamond 4



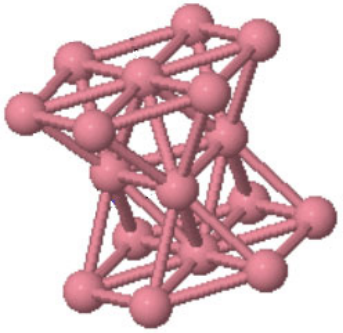
sc 6



bcc 8



fcc 12

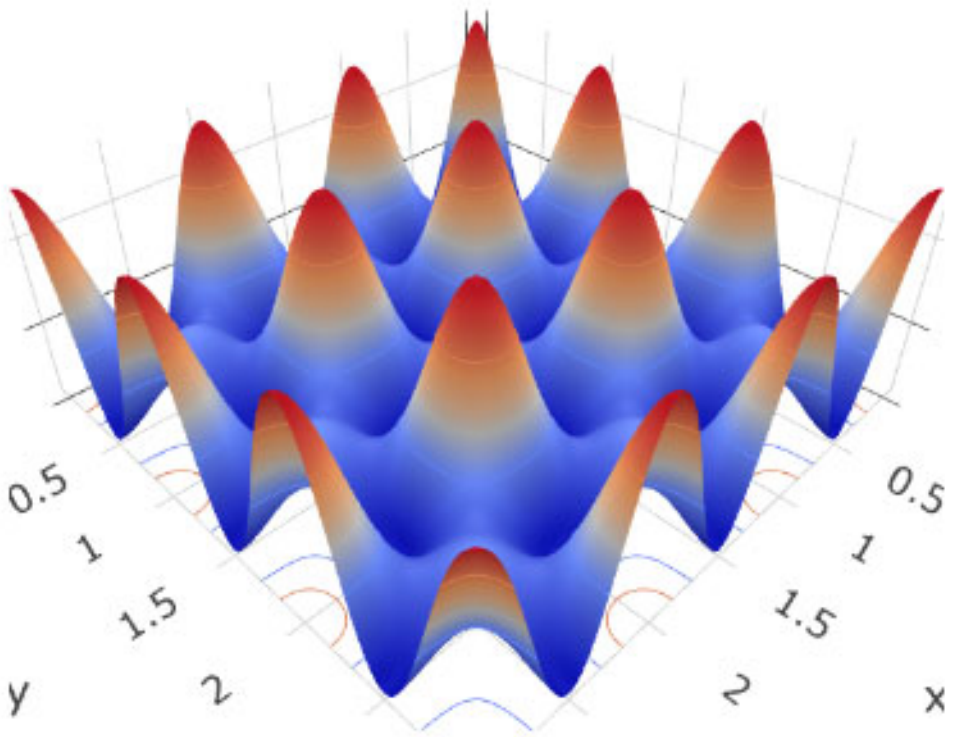


hcp 12

After completing this chapter you should

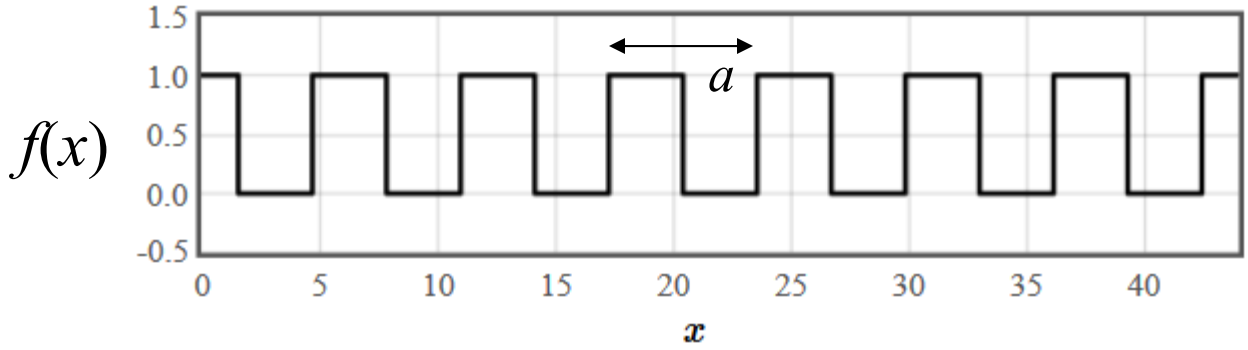
- know that a crystal consists of a basis (the atoms of a primitive unit cell) and one of the 14 Bravais lattices.
- know how to construct a Wigner-Seitz cell for a Bravais lattice and know that it is the primitive unit cell with the maximum symmetry.
- understand how directions and planes are specified by Miller indices.
- be able to calculate the volume of the primitive unit cell $= \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)$, the mass density of a crystal, the distance between any two atoms in the crystal, and the angle determined by any three atoms in the crystal structure.
- be able to search the internet for a CIF file of any known crystal and be able to load the CIF file into a program that displays the positions of the atoms. You should be able to extract the lattice parameters (a, b, c, α, β, γ) and the space group from the CIF file. From the space group, you should be able to determine the Bravais lattice and the point group of the crystal. You should be able to determine how the point group restricts the form of the tensor properties of this crystal.
- know that the basis of a crystal can be constructed by applying the space group symmetries to the asymmetric unit.

Periodic functions



Use a Fourier series to describe periodic functions

Expanding a 1-d function in a Fourier series



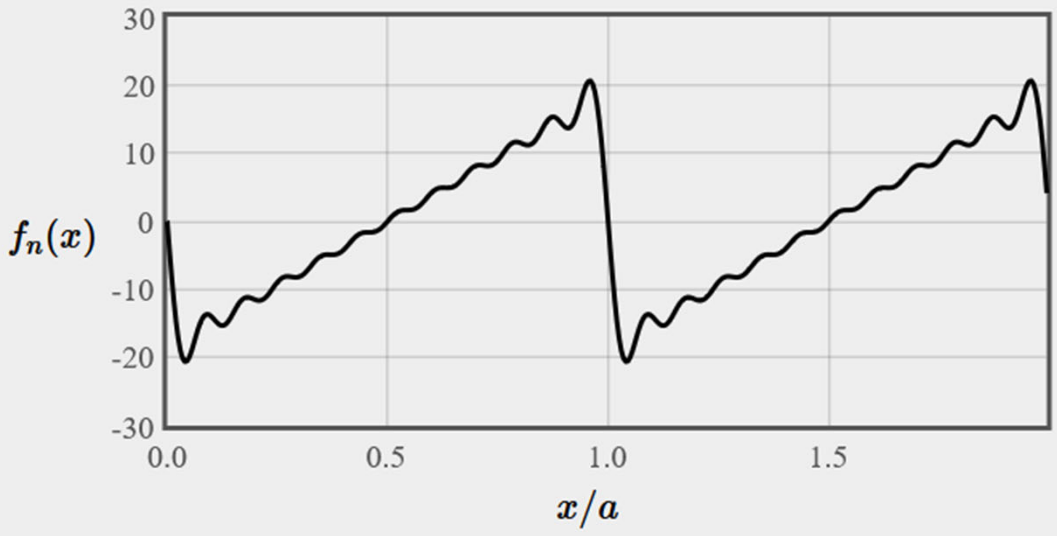
Any periodic function can be represented as a Fourier series.

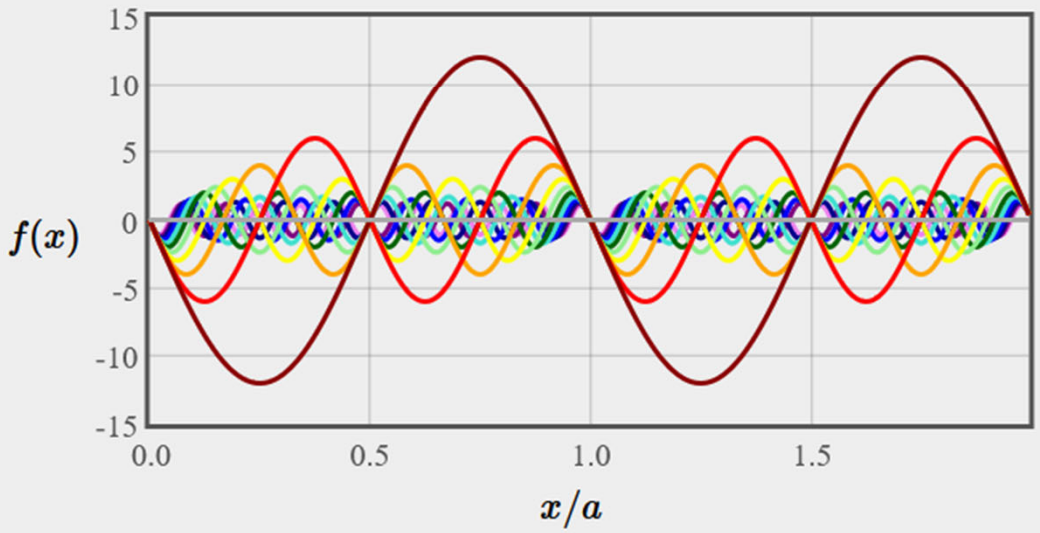
$$f(x) = f_0 + \sum_{p=1}^{\infty} c_p \cos(2\pi px/a) + s_p \sin(2\pi px/a)$$

multiply by $\cos(2\pi p'x/a)$ and integrate over a period.

$$\int_0^a f(x)\cos\left(2\pi p'x/a\right)dx = c_p \int_0^a \cos\left(2\pi p'x/a\right)\cos\left(2\pi p'x/a\right)dx = \frac{ac_{p'}}{2}$$

$$c_p = \frac{2}{a}\int_0^a f(x)\cos\left(2\pi px/a\right)dx$$



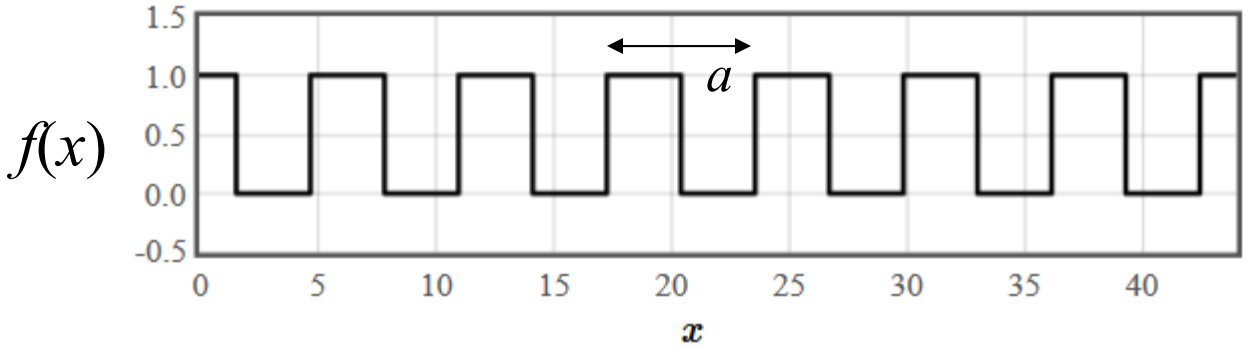


Number of periods displayed: 2

sine | cosine | odd square | even square | triangle

sawtooth | comb | pulse | beats | burst

Expanding a 1-d function in a Fourier series



Any periodic function can be represented as a Fourier series.

$$f(x) = f_0 + \sum_{p=1}^{\infty} c_p \cos(2\pi px/a) + s_p \sin(2\pi px/a)$$

$$\cos x = \frac{e^{ix} + e^{-ix}}{2} \qquad \sin x = \frac{e^{ix} - e^{-ix}}{2i}$$

$$f(x) = \sum_{G=-\infty}^{\infty} f_G e^{iGx} \qquad f_G = \frac{c_p}{2} - i\frac{s_p}{2} \qquad G = \frac{2\pi p}{a}$$

For real functions: $f_G^* = f_{-G}$

reciprocal lattice vector