ECE-305: Spring 2018

Material Properties

Pierret, *Semiconductor Device Fundamentals* (SDF)
Chapter 1 (pp. 3-19)
Chapter 2 (pp. 22-32)

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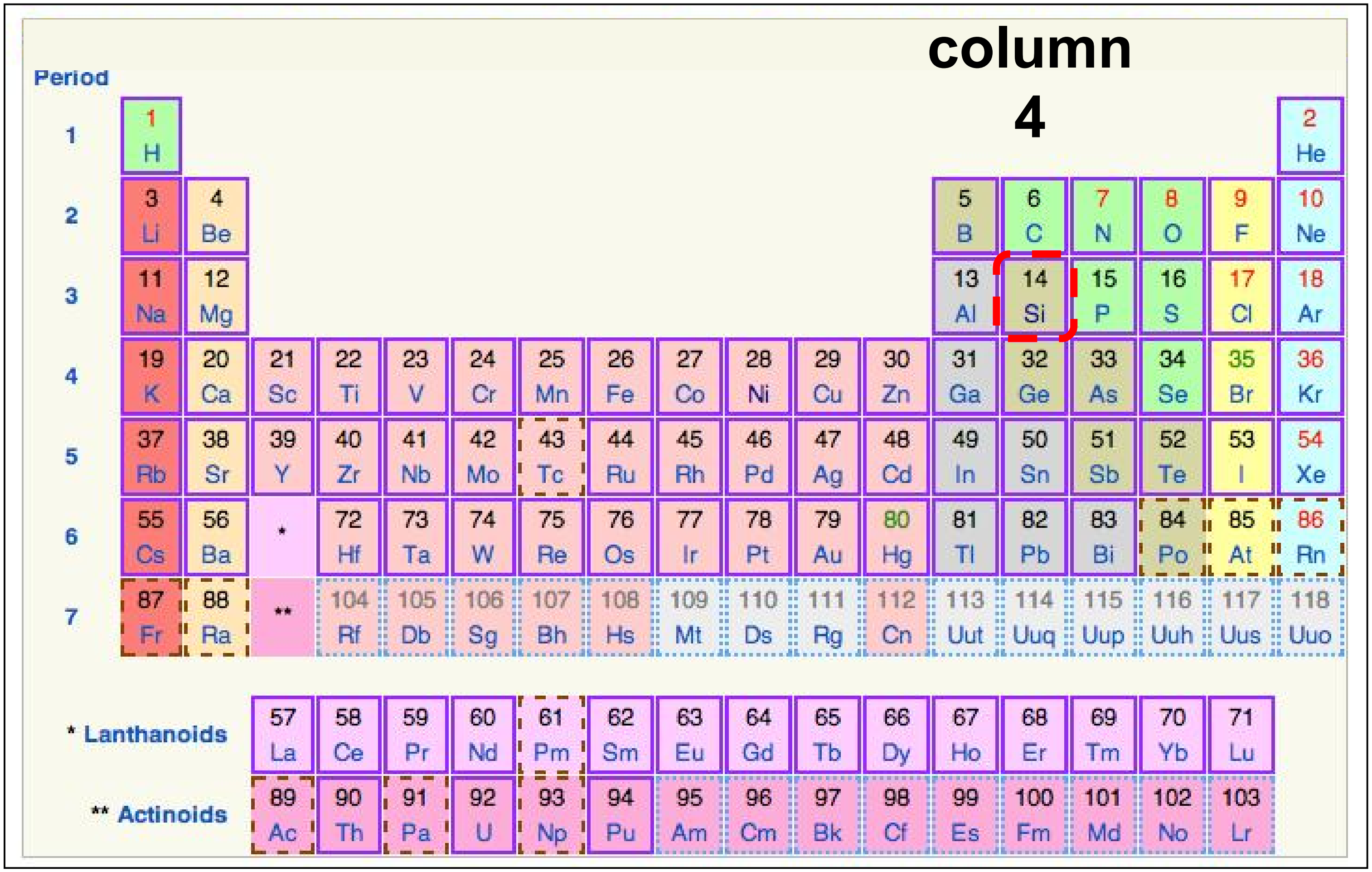
PURDUE UNIVERSITY

outline

1. Graphene
2. Silicon
3. Miller indices
4. Quantization of energy levels
5. Energy bands
6. Electrons and holes
7. Intrinsic carriers
8. Doping

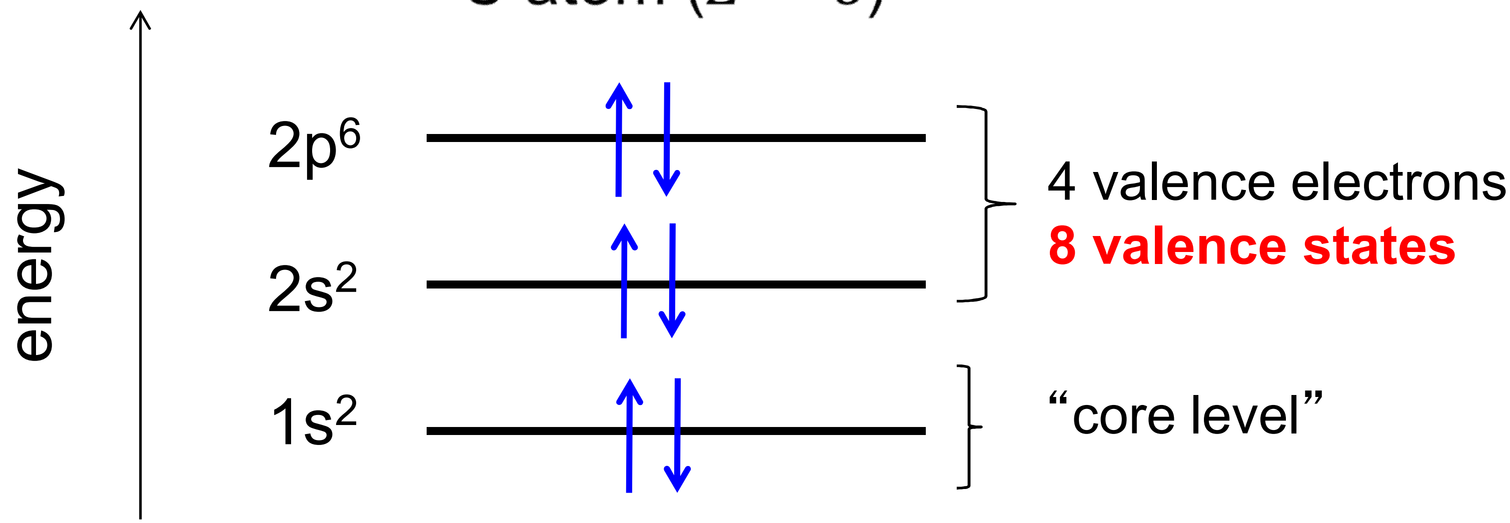
semiconductors

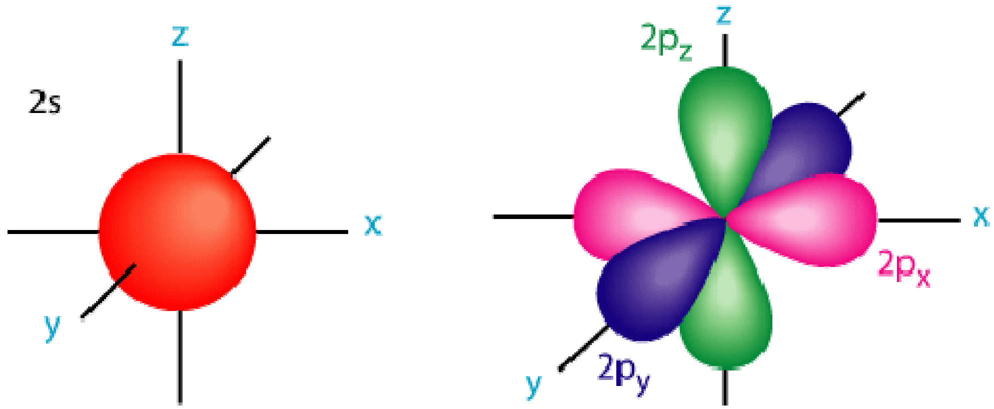


http://en.wikipedia.org/wiki/Periodic_table

carbon energy levels

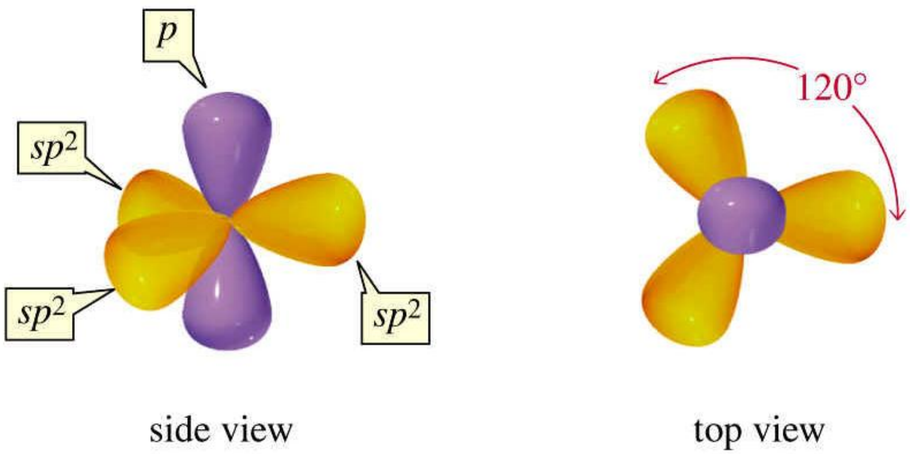
C atom ($Z = 6$)

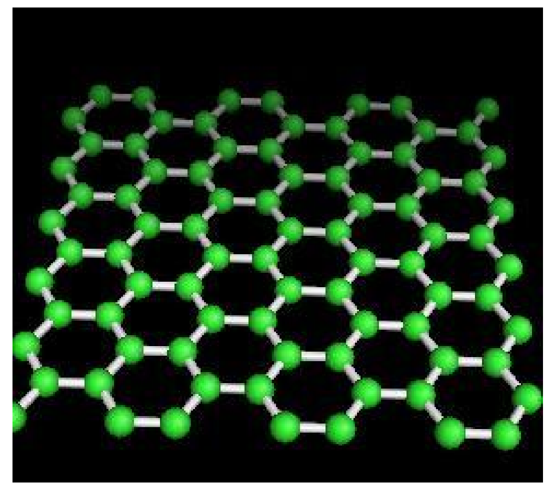




Graphene: 2011 Nobel Prize in Physics

Graphene is a one-atom-thick planar *crystalline* carbon sheet with a triangular lattice with 2 atoms per unit cell.

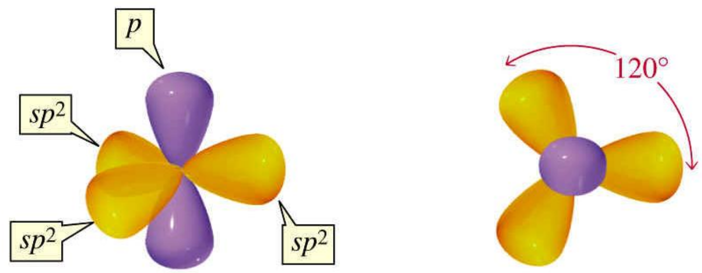


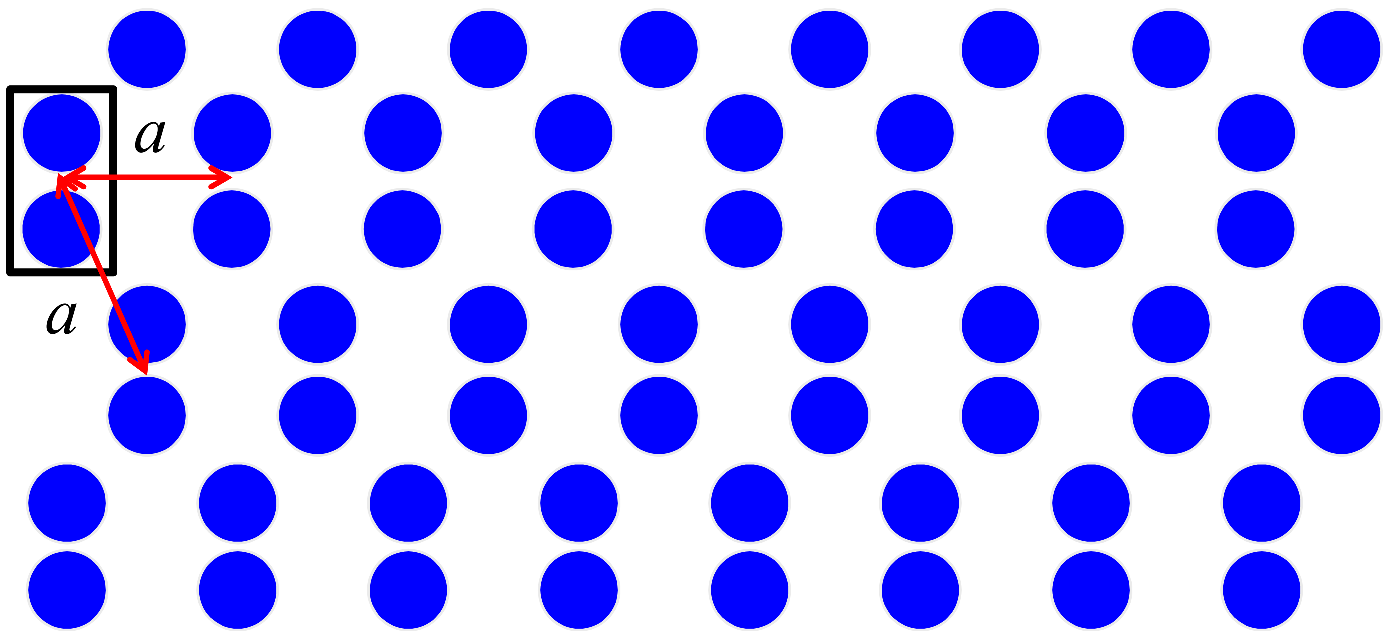


source: CNTBands 2.7.2

https://nanohub.org/resources/1838

triangular lattice + 2 atom basis





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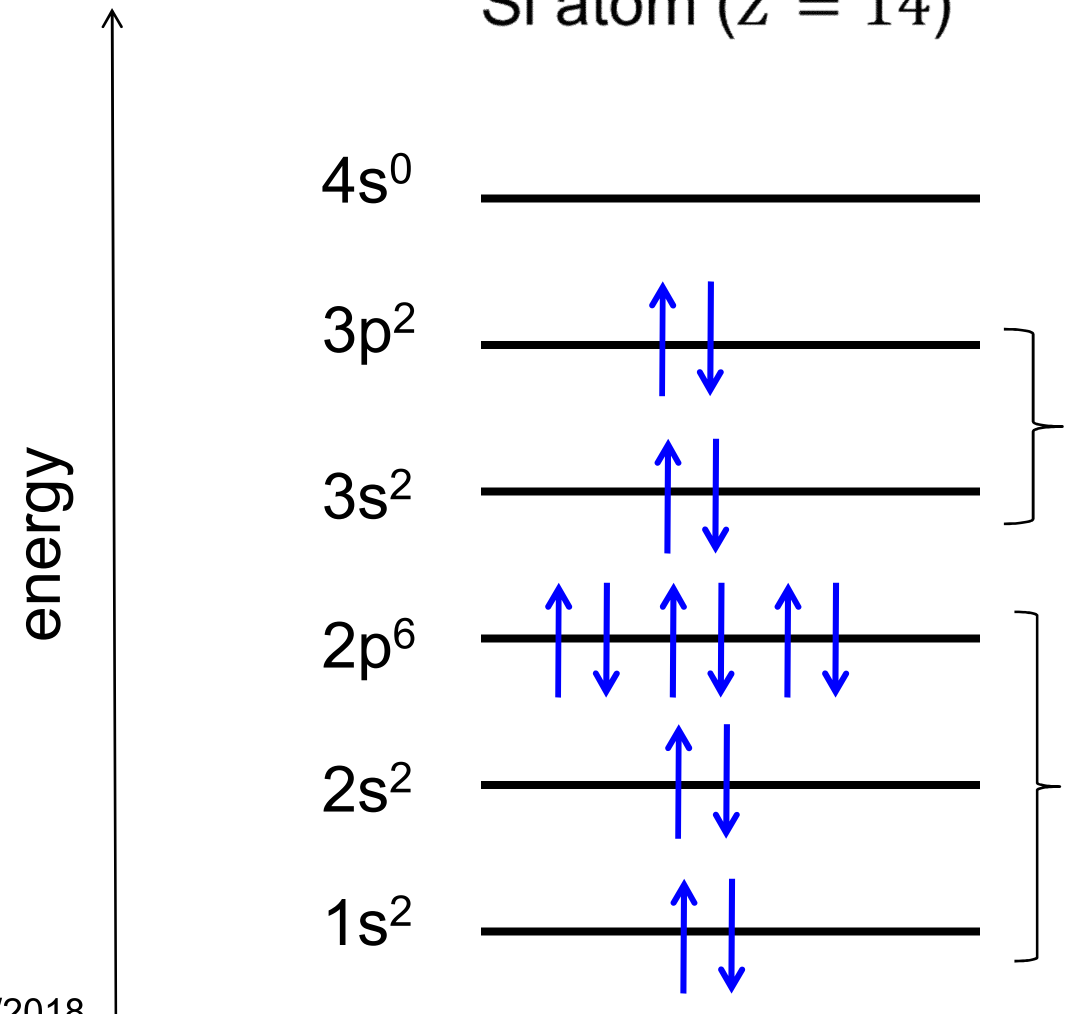
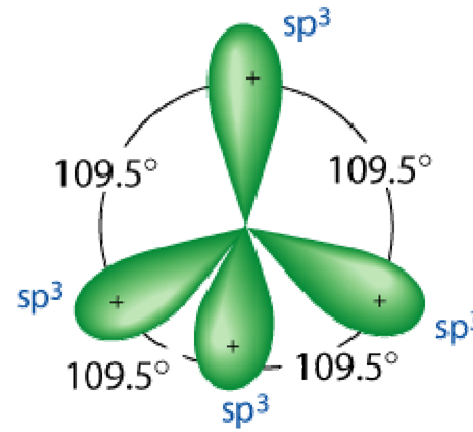
silicon energy levels

Si atom ($Z = 14$)



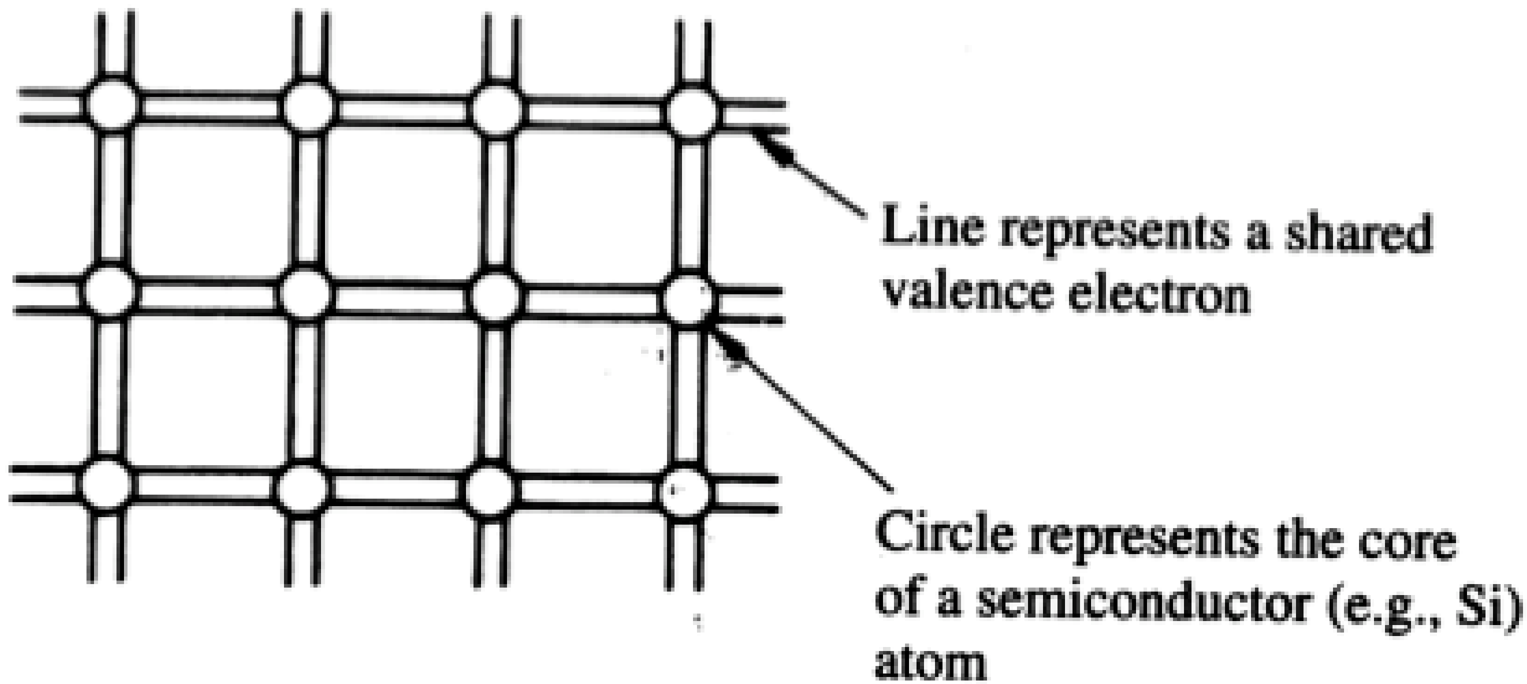


4 valence electrons

8 valence states

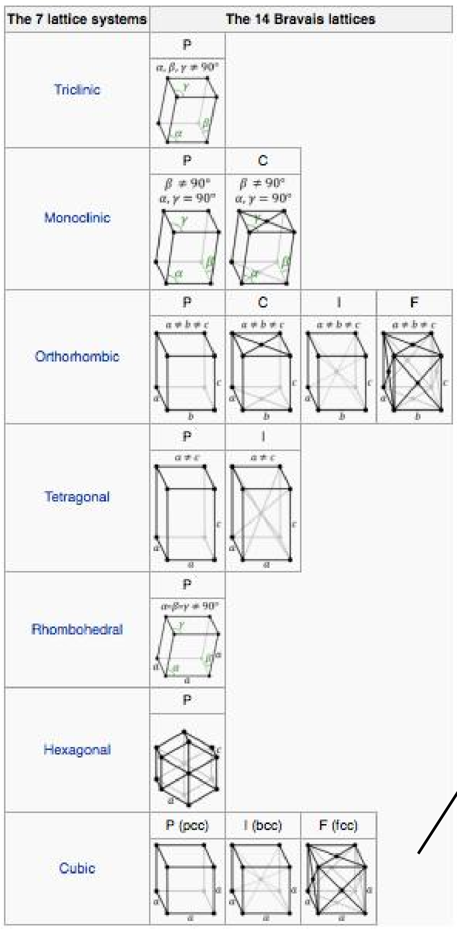
"core levels"

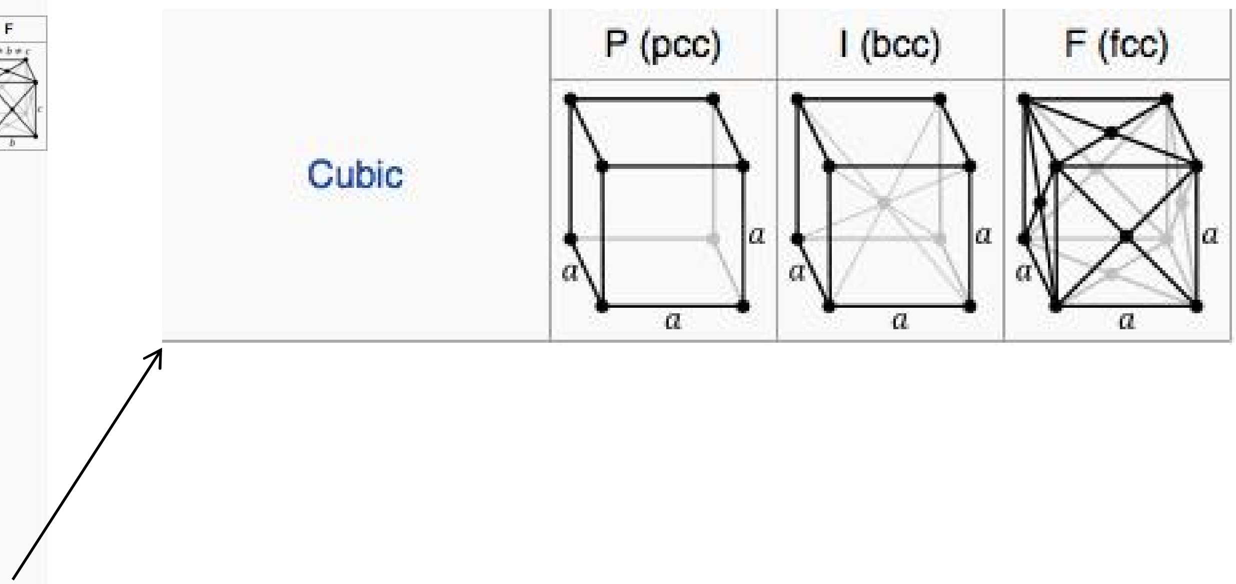
“cartoon” Si crystal



What would you get from combining carbon in the same way?

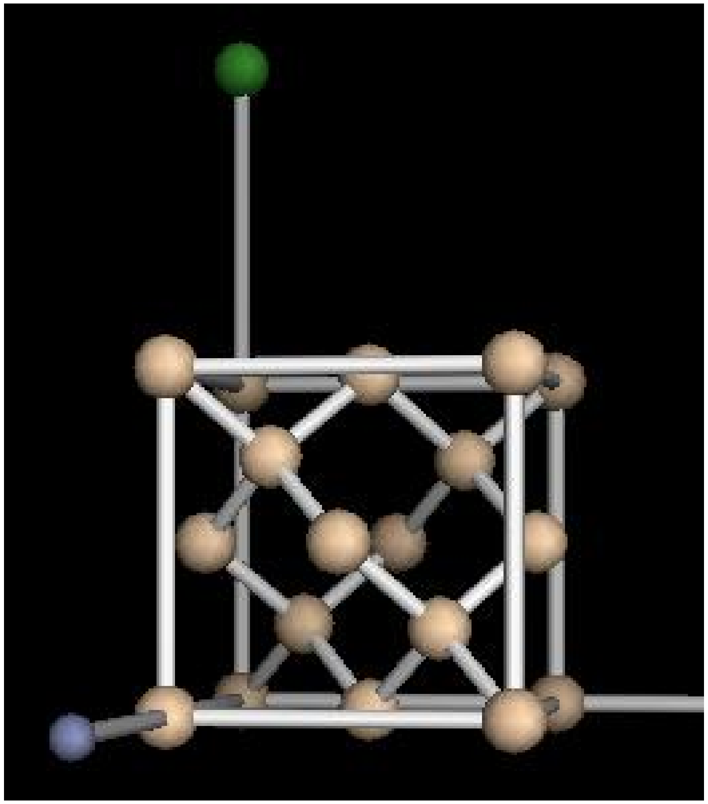
3D crystal structure





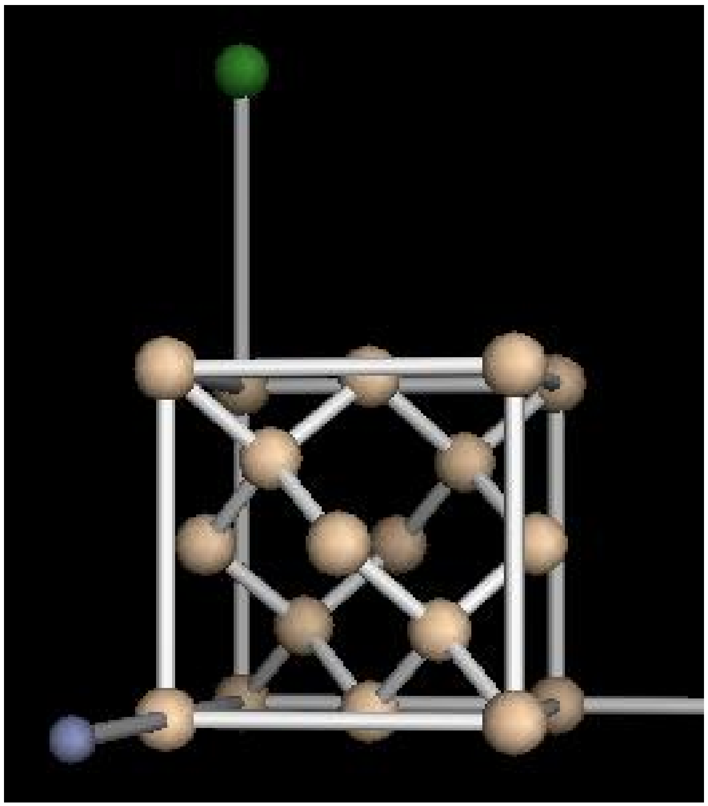
http://en.wikipedia.org/wiki/Bravais_lattice

silicon in diamond lattice



https://nanohub.org/tools/crystal_viewer

The diamond lattice



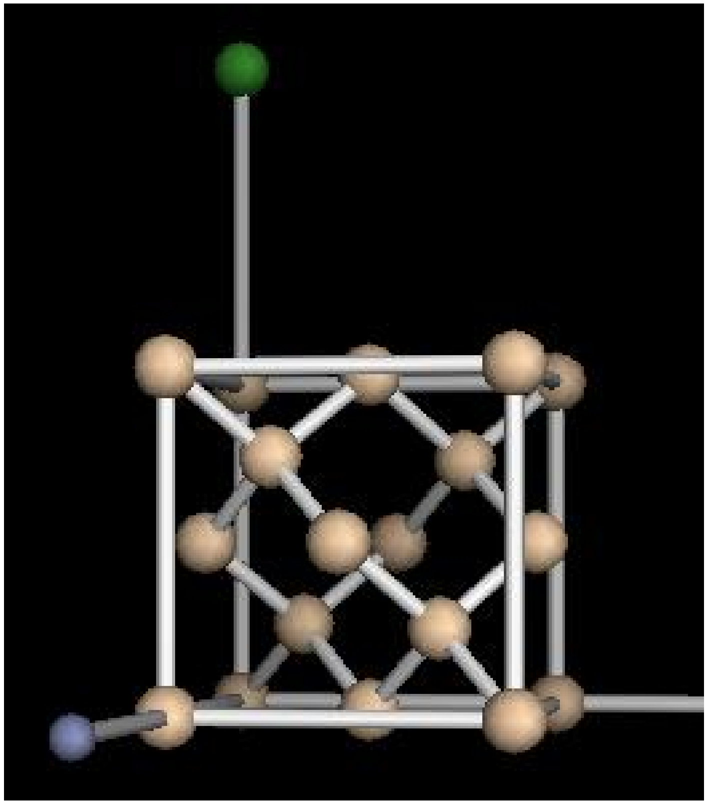
Atoms per unit cell

8 times 1/8 + 6 times ½ + 4

8 atoms per unit cell

https://nanohub.org/tools/crystal_viewer

Silicon: nearest neighbor (NN) spacing



Lattice constant: $a = 5.4307$ Å

Body diagonal = $a\sqrt{3}$.

NN spacing = $a\sqrt{3}/4$

https://nanohub.org/tools/crystal_viewer

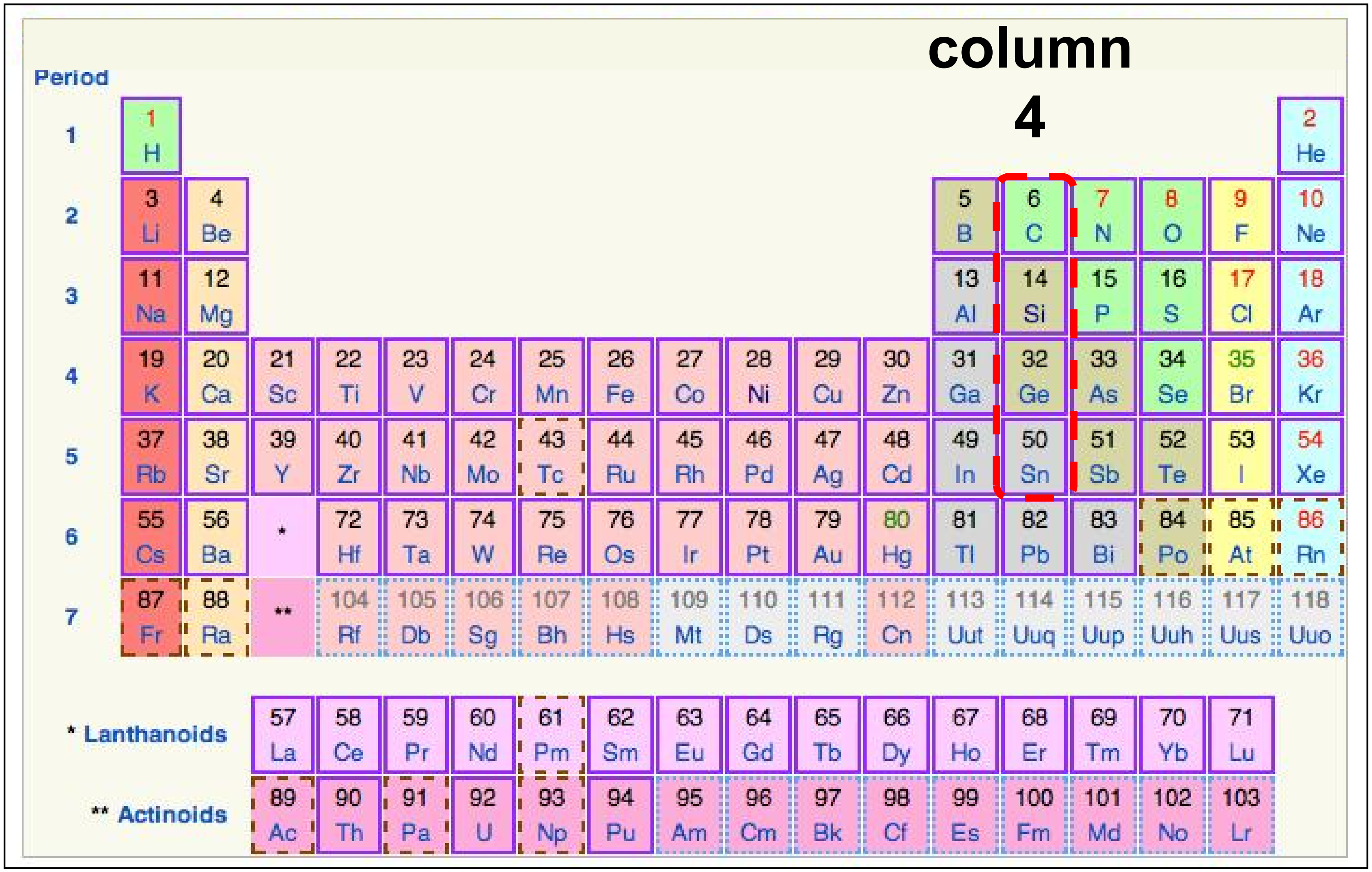
Si atoms in a solid

1) In a Si **crystal**, each atom occupies, a specific location in a crystal lattice.

2) **Polycrystalline** Si consider of many crystalline “grains” with different orientations.

3) In **amorphous** Si, the atoms are more or less randomly distributed throughout the solid.

semiconductors



Period																		
1	1 H																	2 He
2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
3	11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba	*	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra	**	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Uut	114 Uuq	115 Uup	116 Uuh	117 Uus	118 Uuo

* Lanthanoids	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
** Actinoids	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

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semiconductors

Col. 3 Col. 5

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5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
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7	87 Fr	88 Ra	**	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Uut	114 Uuq	115 Uup	116 Uuh	117 Uus	118 Uuo

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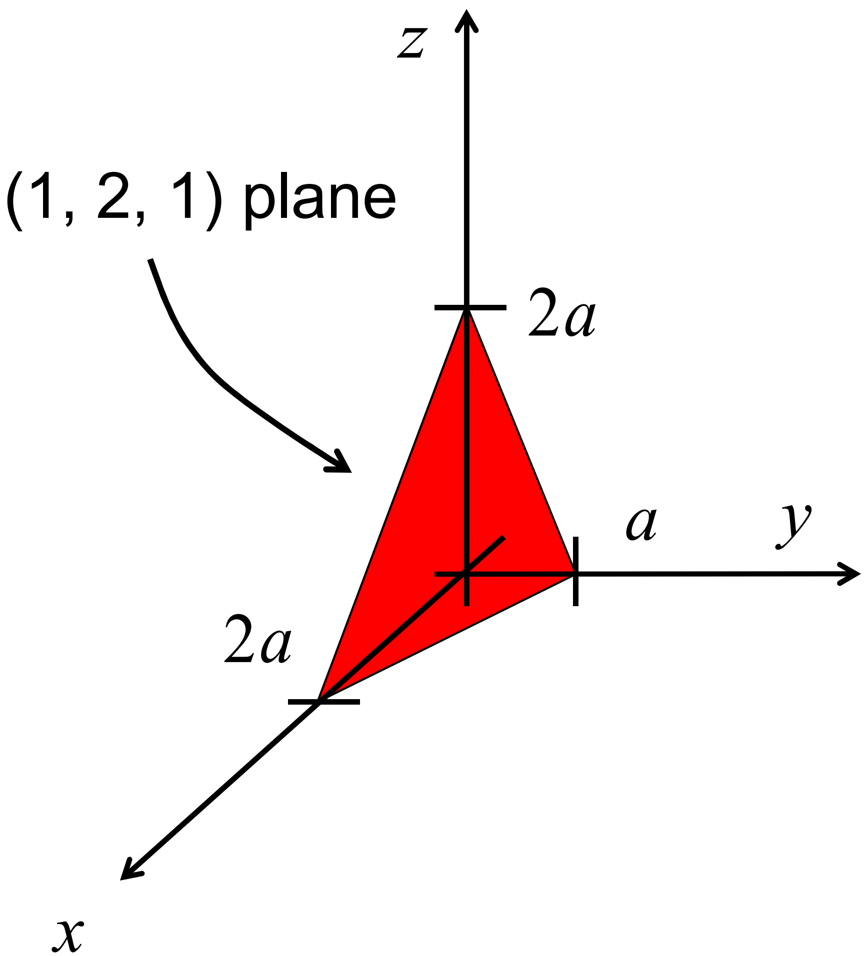
Miller index prescription for describing planes



x, y, and z-axis intercepts:

2a, 1a, 2a
2, 1, 2

invert:

½. 1, ½

Rationalize:

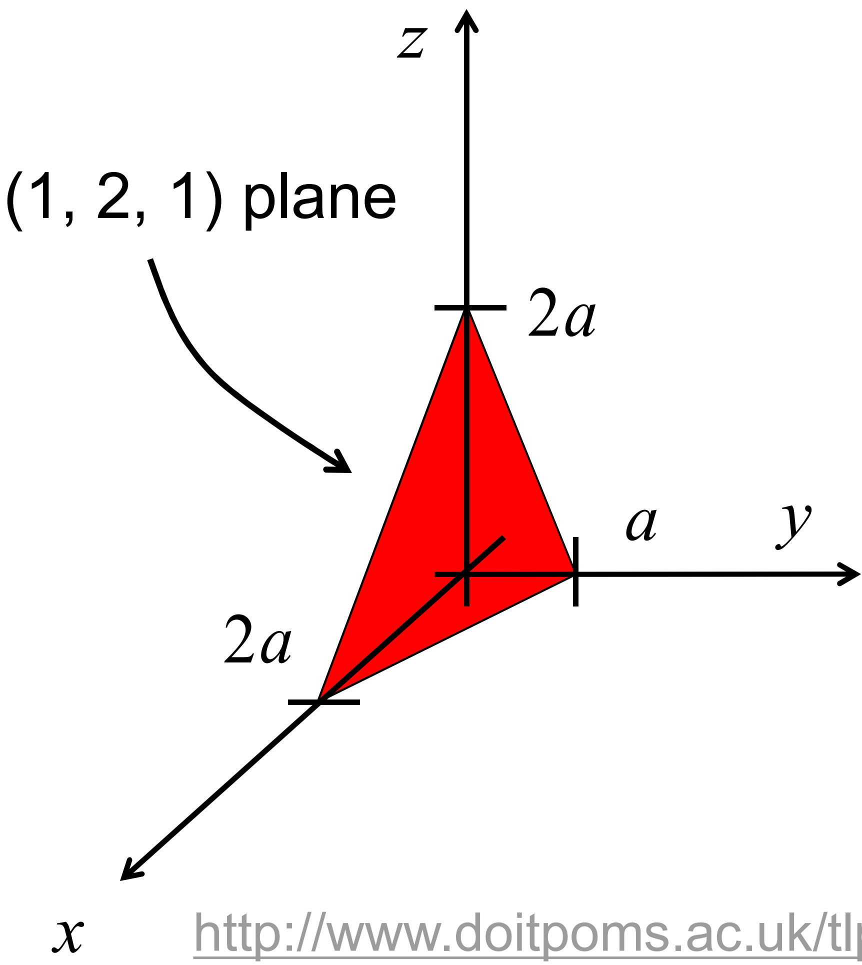
1, 2, 1

question

Where does this prescription come from?

Answer: If we remember the equation for a plane, we can figure it out.

where it comes from



equation of a plane:

$$\frac{x}{x_{\text{int}}}+\frac{y}{y_{\text{int}}}+\frac{z}{z_{\text{int}}}=1$$

describe with the numbers:

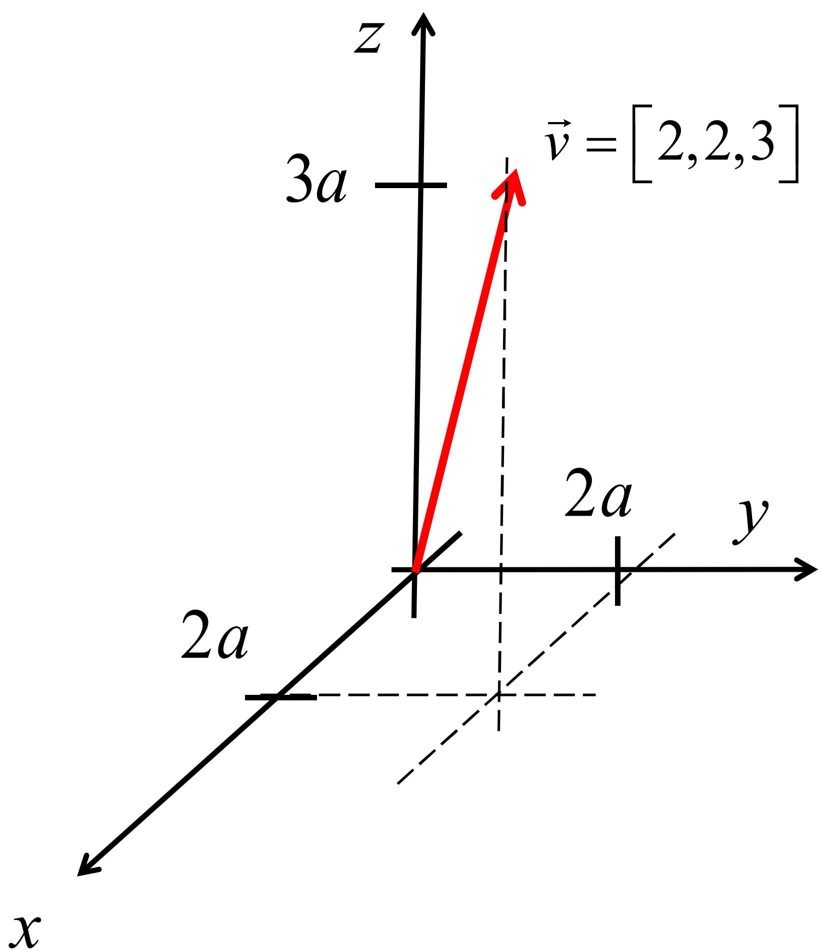
$$\frac{1}{x_{\text{int}}},\frac{1}{y_{\text{int}}},\frac{1}{z_{\text{int}}}$$

equivalent to:

$$\frac{1}{x_{\text{int}}/a},\frac{1}{y_{\text{int}}/a},\frac{1}{z_{\text{int}}/a}$$

http://www.doitpoms.ac.uk/tlplib/miller_indices/lattice_draw.php

prescription for describing directions



equation of a vector:

$$\vec{v} = 2a\hat{x} + 2a\hat{y} + 3a\hat{z}$$

describe with components:

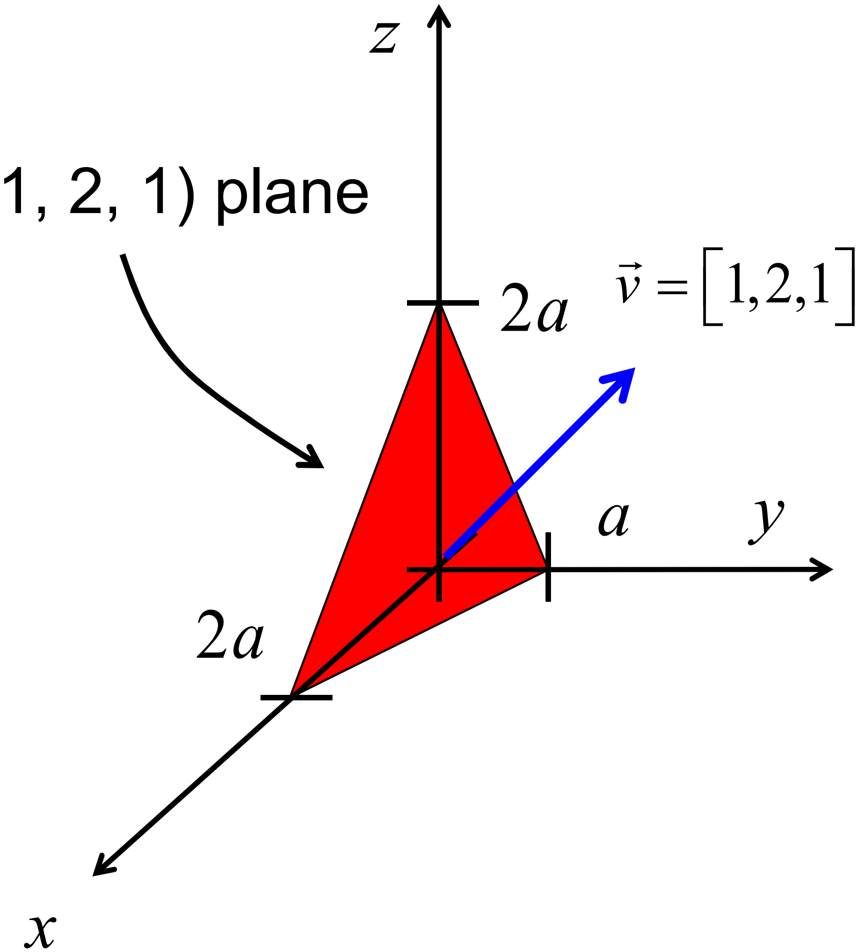
$$2a, 2a, 3a$$

equivalent to:

$$2,2,3$$

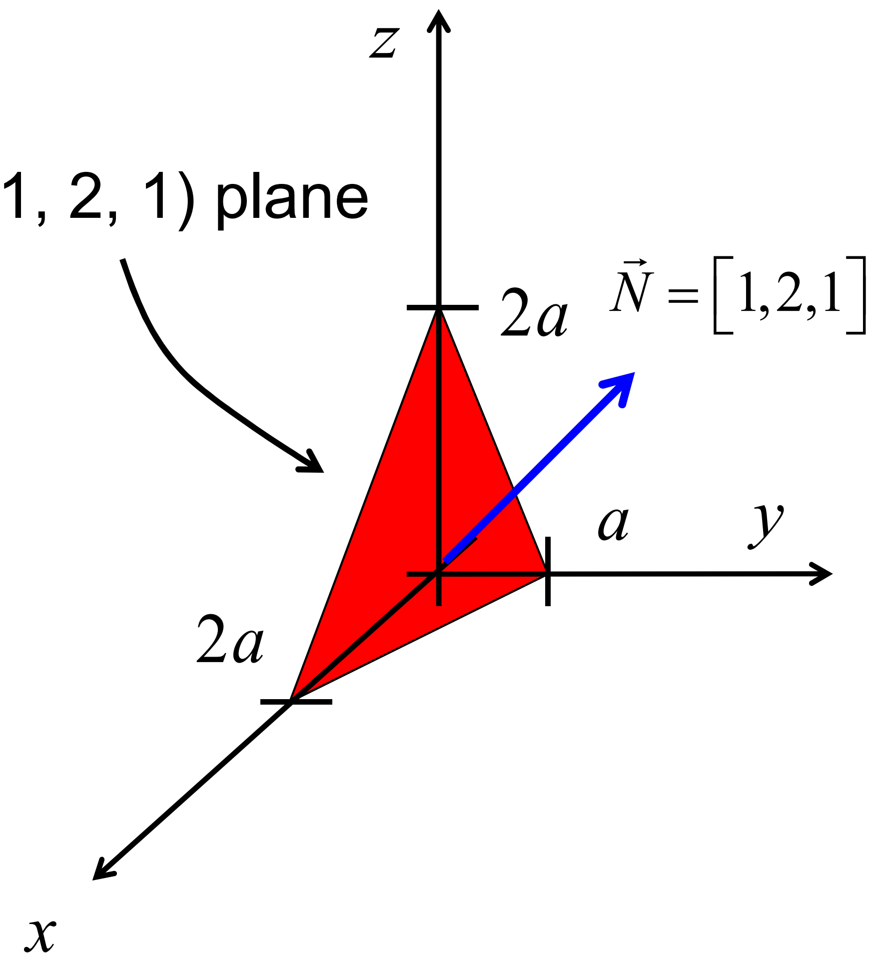
direction normal to a plane

(1, 2, 1) plane



Why is [1, 2, 1] normal to (1, 2, 1)?

where it comes from



equation of a plane:

$$f\left(x,y,z\right) = \frac{x}{x_{\text{int}}} + \frac{y}{y_{\text{int}}} + \frac{z}{z_{\text{int}}} = 1$$

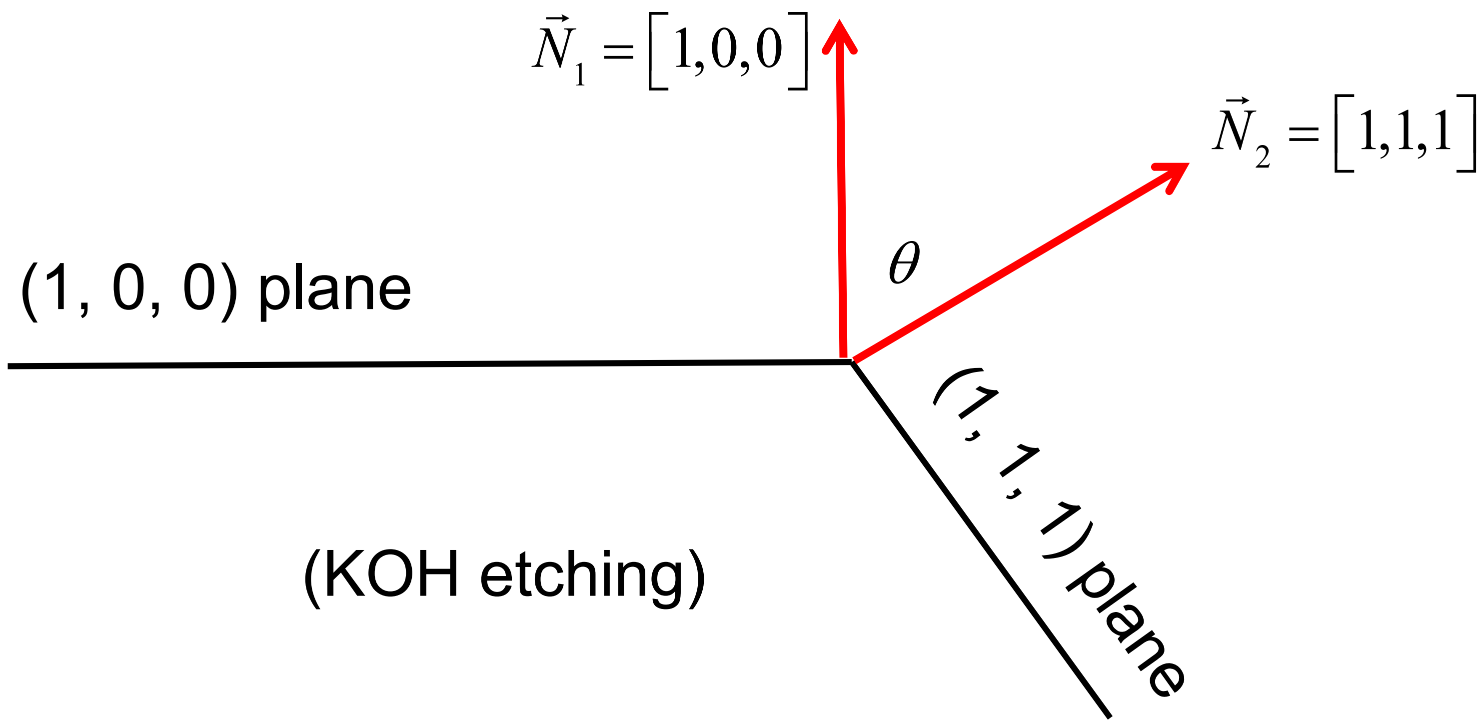
normal to a plane:

$$\vec{N} = \nabla f\left(x,y,z\right) = \frac{\partial f}{\partial x}\hat{x} + \frac{\partial f}{\partial y}\hat{y} + \frac{\partial f}{\partial x}\hat{z}$$

(gradient)

$$\vec{N} = \frac{1}{x_{\text{int}}}\hat{x} + \frac{1}{y_{\text{int}}}\hat{y} + \frac{1}{z_{\text{int}}}\hat{z}$$

angle between planes



$$\vec{N}_1 \bullet \vec{N}_2 = N_1 N_2 \cos\theta$$

angle between planes

$$\cos\theta = \frac{\vec{N}_1 \bullet \vec{N}_2}{N_1 N_2}$$

$$\vec{N}_1 = \left[h_1, k_1, l_1\right]$$

$$\vec{N}_2 = \left[h_2, k_2, l_2\right]$$

$$\cos\theta = \frac{h_1 h_2 + k_1 k_2 + l_1 l_2}{\sqrt{h_1^2 + k_1^2 + l_1^2}\sqrt{h_2^2 + k_2^2 + l_2^2}}$$

$$\vec{N}_1 = \left[1,0,0\right]$$

$$\vec{N}_2 = \left[1,1,1\right]$$

$$\cos\theta = \frac{1+0+0}{\sqrt{1^2 + 0^2 + 0^2}\sqrt{1_2^2 + 1_2^2 + 1_2^2}}$$

$$\cos\theta = \frac{1}{\sqrt{3}}$$

$$\theta = 54.7^\circ$$

summary

$\left(h\ k\ l\right)$ A specific plane.

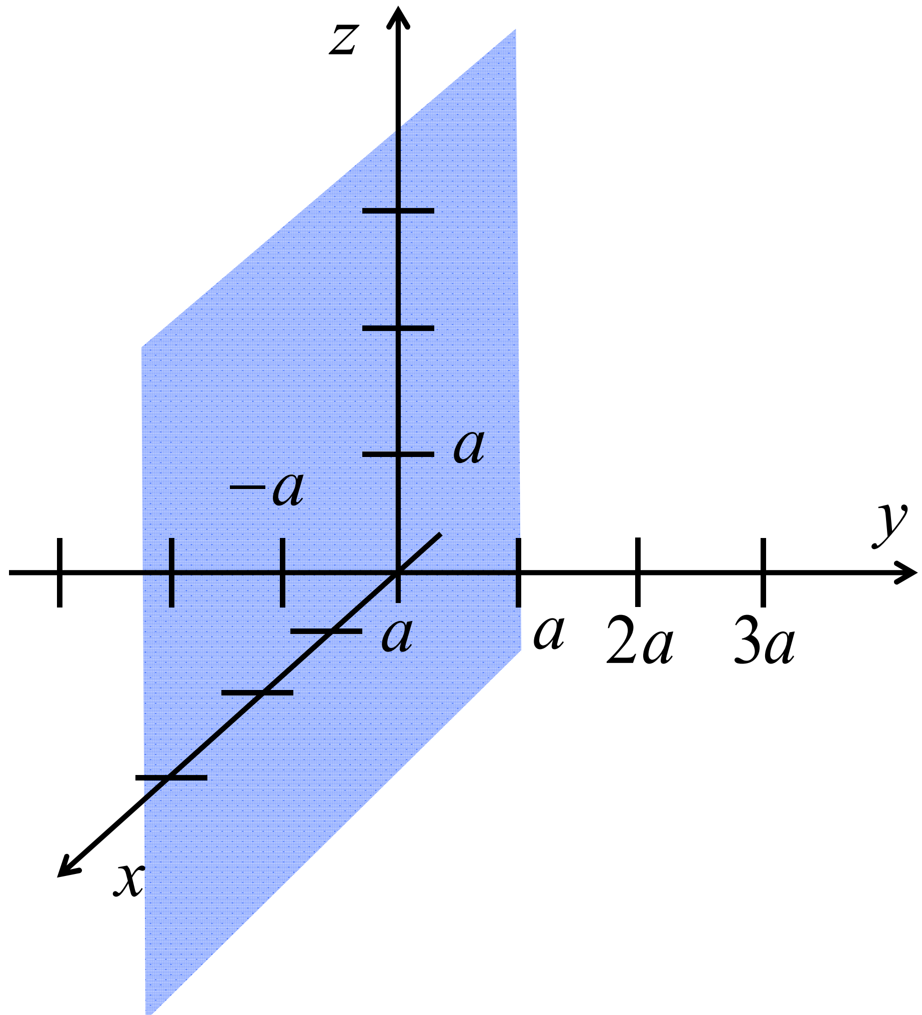
$\left[h\ k\ l\right]$ A direction normal to the plane above.

$$\vec{N} = ha\hat{x} + ka\hat{y} + la\hat{z}$$

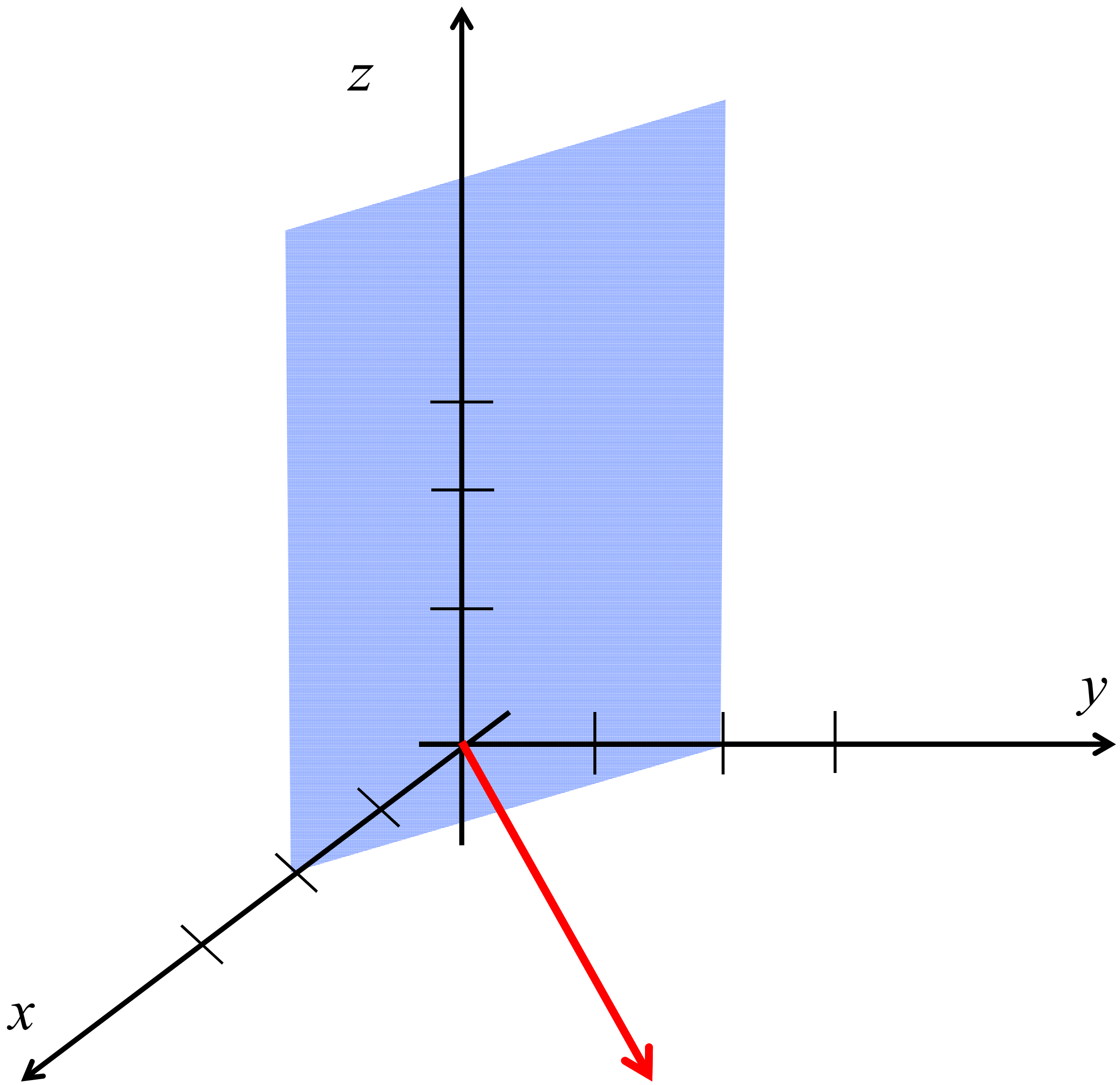
$\left\{h\ k\ l\right\}$ A set of equivalent planes.

$\left\langle h\ k\ l\right\rangle$ A set of equivalent directions.

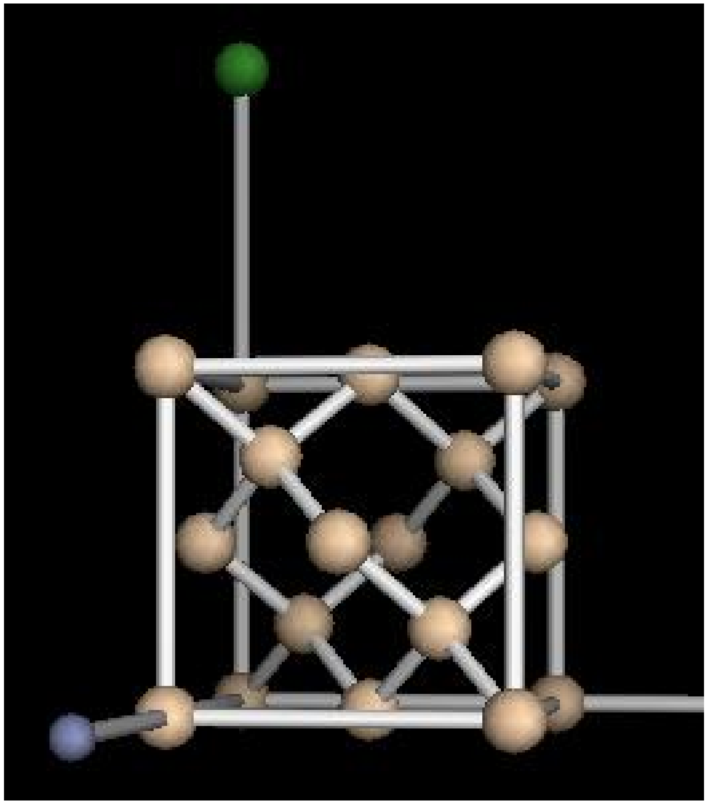
what plane is this?



what plane is this?



Silicon: atoms / cm^2 on (100)



Lattice constant: 5.4307 Ang

Atoms on face = 4 times ¼ +1 = 2

$Ns = 2/a^2$

$Ns = 6.81x\ 10^{14}\ /cm^2$

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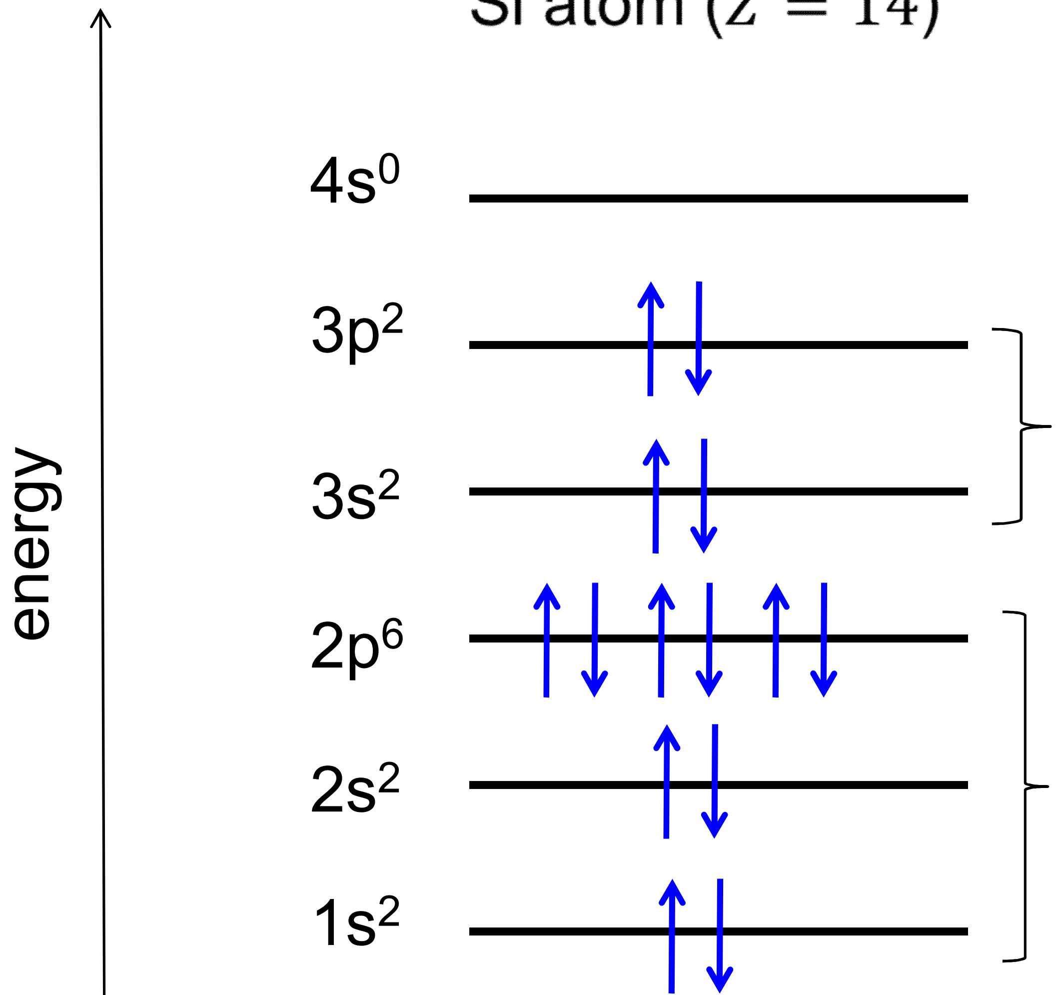
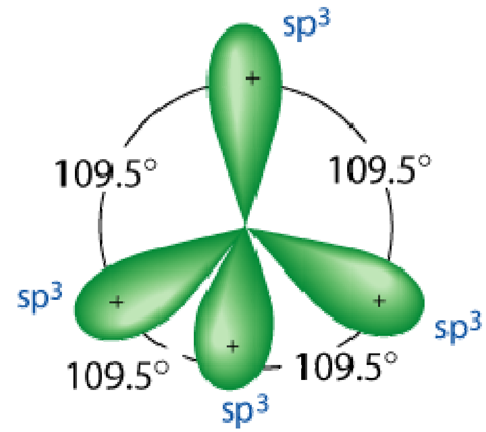
silicon energy levels

Si atom ($Z = 14$)





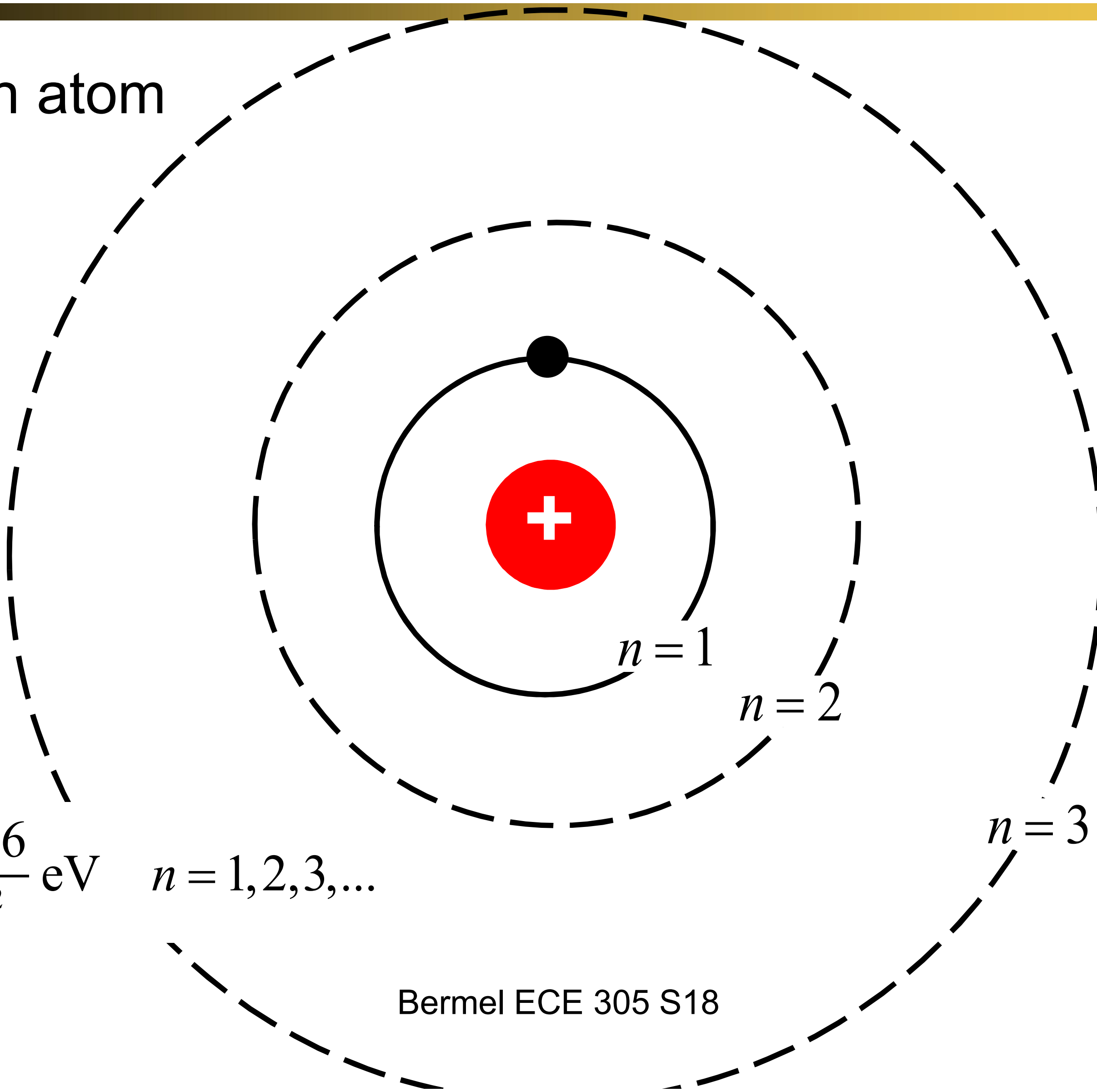
4 valence electrons

8 valence states

“core levels”

quantization of energy levels

Hydrogen atom



$$E_H = -\frac{13.6}{n^2}\ \text{eV} \quad n = 1, 2, 3, \ldots$$

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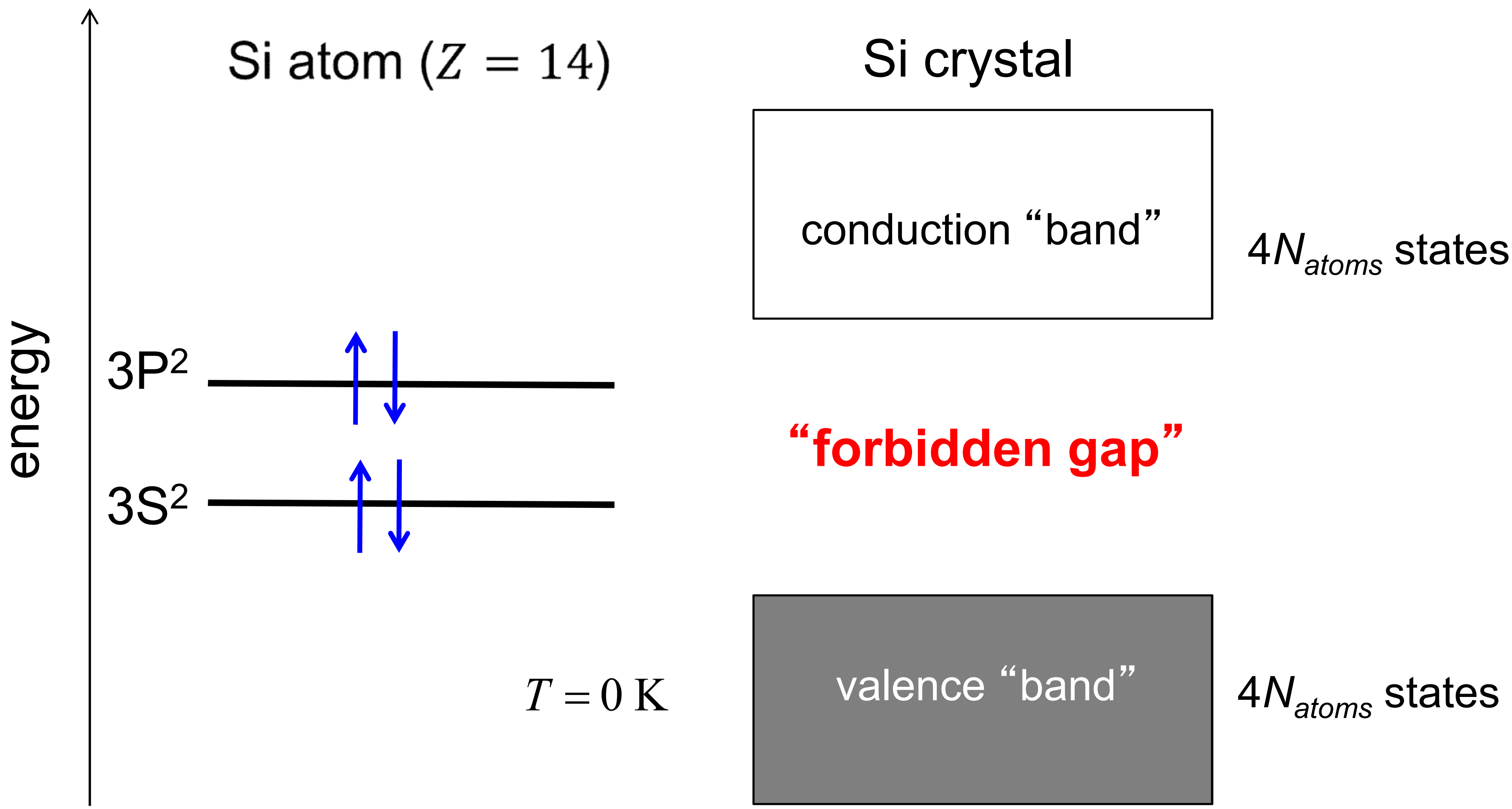
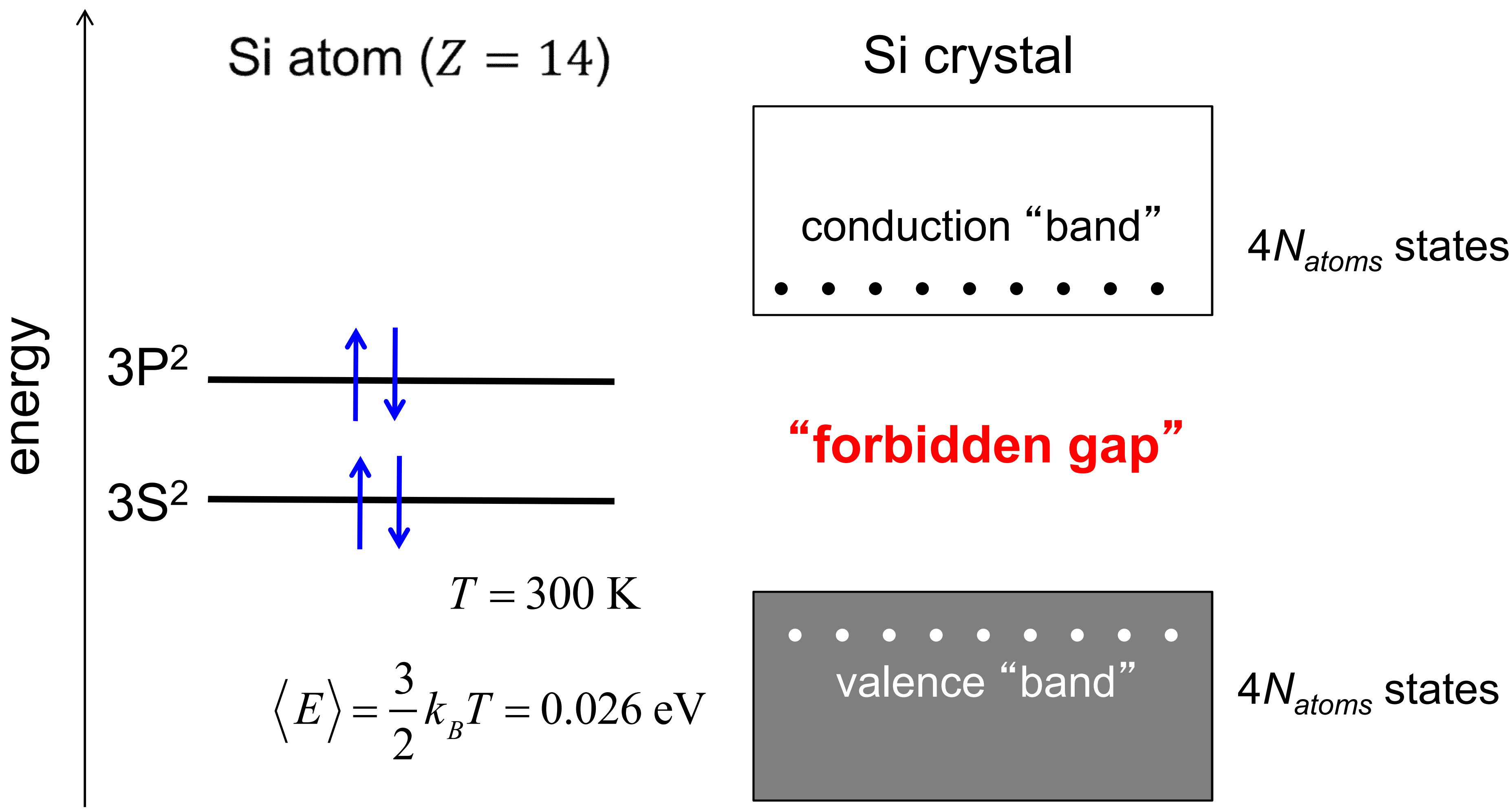
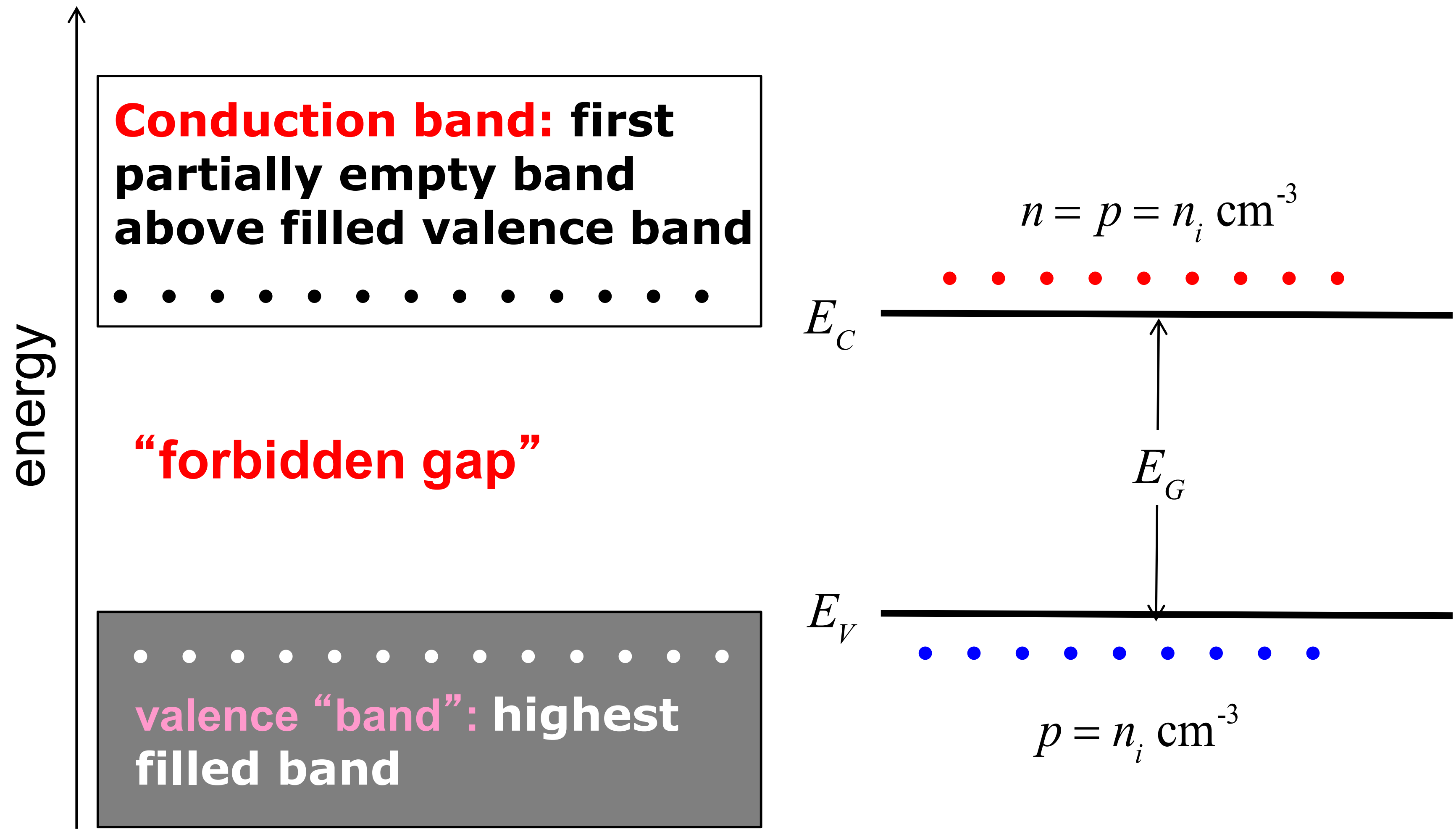
silicon energy levels → energy bands



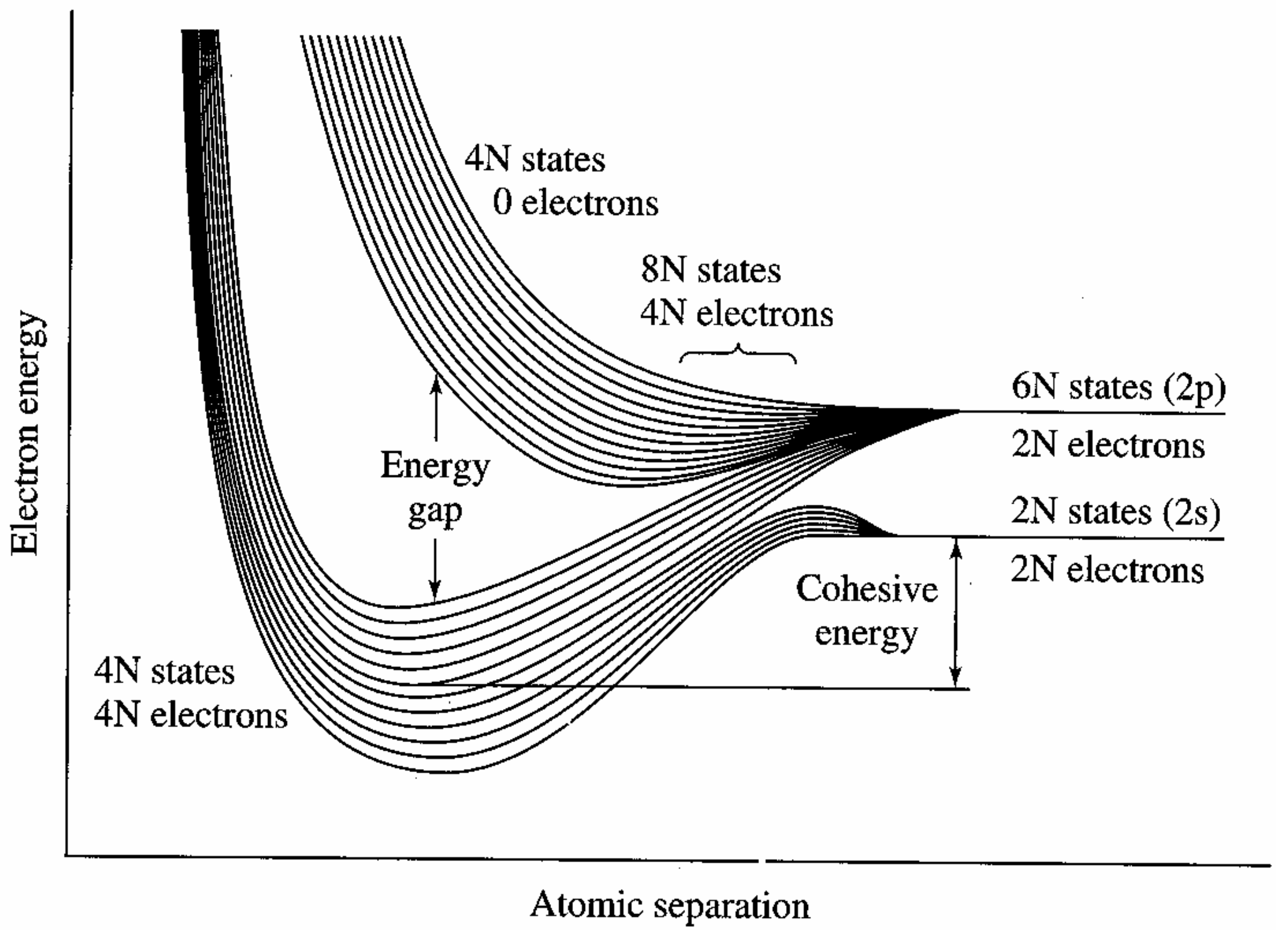
silicon energy levels → energy bands



energy band diagrams



energy bands versus atomic separation



Si atoms
$1s^2 2s^2 2p^6 3s^2 2p^2$
C atoms
$1s^2 2s^2 2p^2$

2s – 2 states
2p – 6 states

For N atoms:

2s line –
2N-fold degenerate

2p line –
6N-fold degenerate

insulators metals semiconductors

don't conduct electricity well

<u>do</u> conduct electricity well

in-between, **but** can be controlled

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summary

1. Most solid materials are crystals, which fill space with periodically repeated elements
2. Showed how atomic energy level quantization leads to energy band formation in materials
3. Three types of materials: insulators, metals, and semiconductors