ECE 340 Lecture 4
Semiconductor Electronics

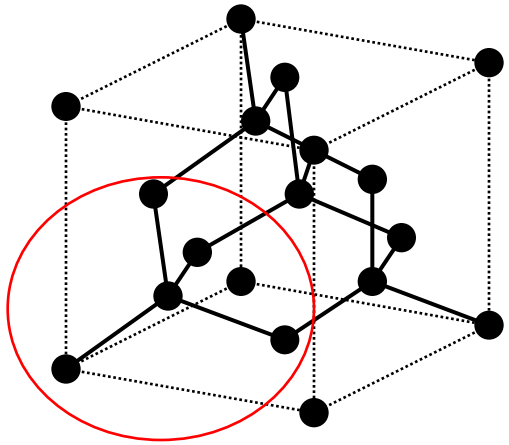
Spring 2022
10:00-10:50am
Professor Umberto Ravaioli
Department of Electrical and Computer Engineering
2062 ECE Building

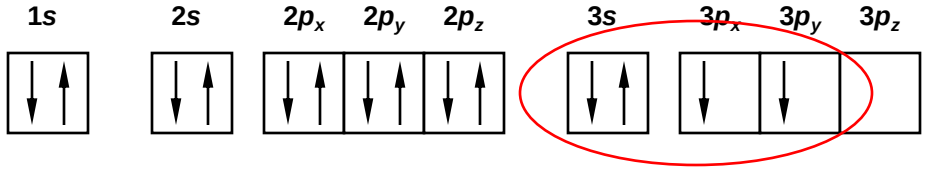
Today's Discussion

- Crystal States
- Types of Bonding
- Insulators, Metals, and Semiconductors
- Band structure
- Direct and Indirect Band Gap
- Electrons and Holes

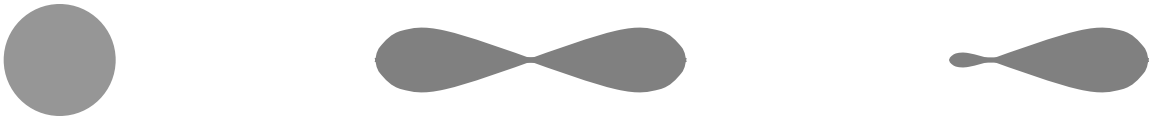
Crystal Bonding

- Each atom shares bonds with 4 other atoms.
- Silicon bonds are covalent, but compound semiconductors have a mix of ionic and covalent bonds.





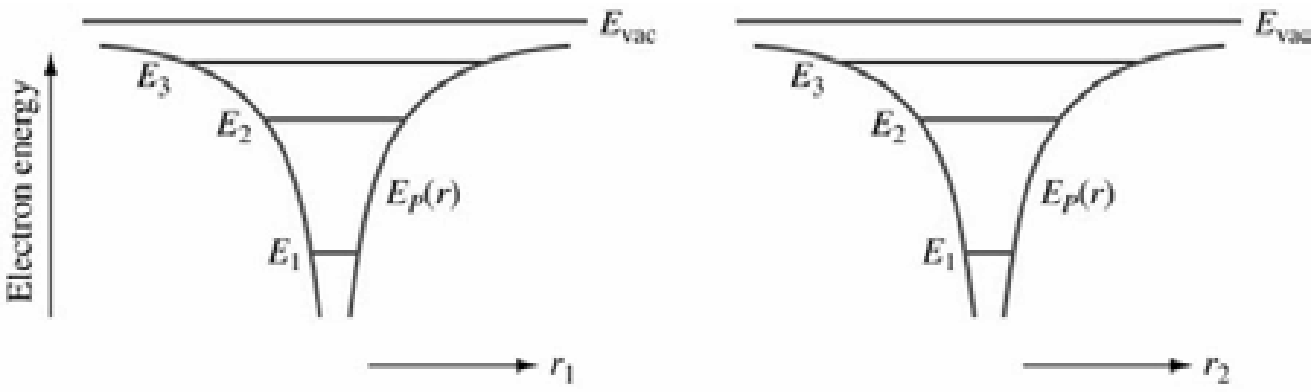
When silicon atoms COMBINE to form a crystal the *s*- and *p*- orbitals HYBRIDIZE to form so-called sp^3 ORBITALS that are mixtures of the *s*- and *p*-orbitals.

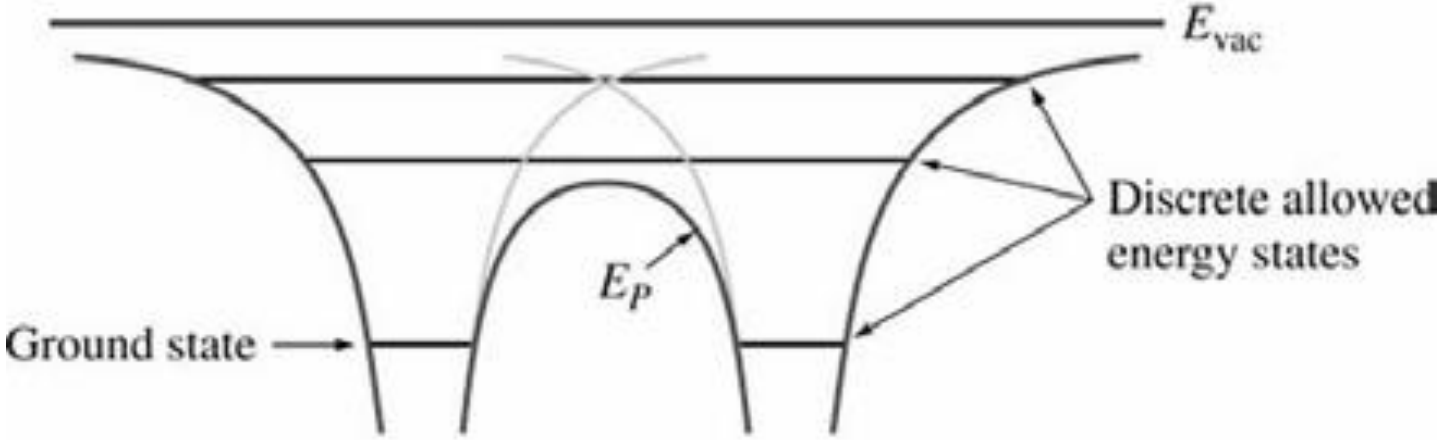


s-ORBITAL | *p*-ORBITAL | sp^3-ORBITAL

Crystal Bonding

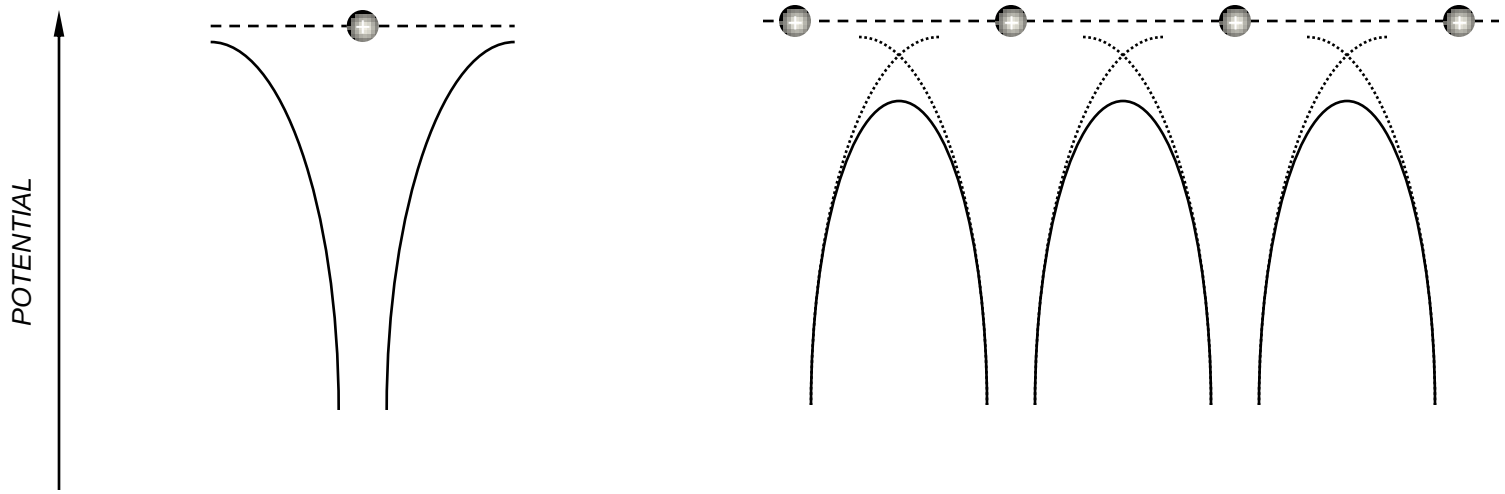
Bring atoms together, the wavefunctions begin to overlap.





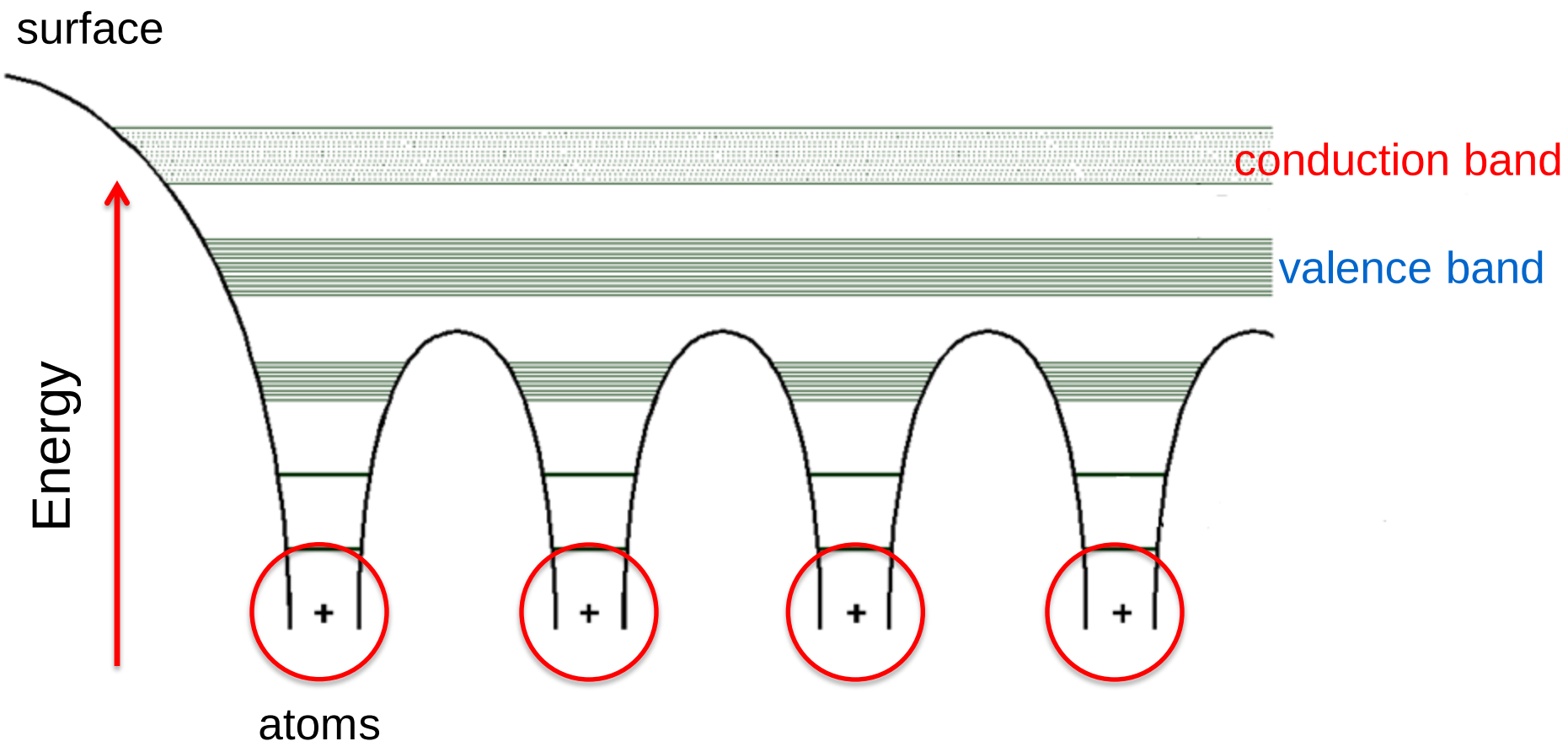
Energy Band Formation

IN A SINGLE ATOM ELECTRONS ARE TRAPPED IN A POTENTIAL WELL

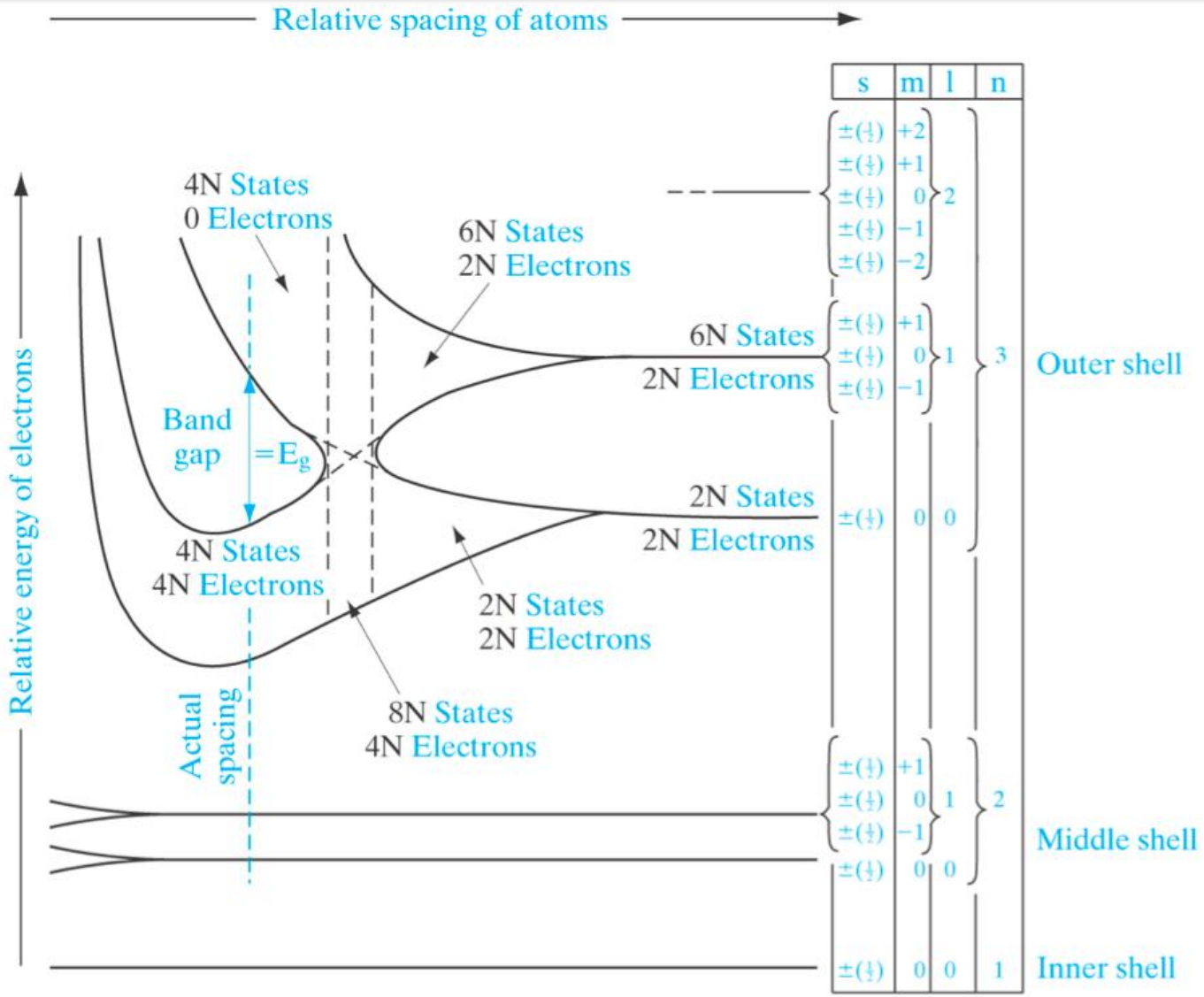


WHEN MANY ATOMS COMBINE AND FORM A CRYSTAL THE ATOMIC POTENTIALS OVERLAP GIVING RISE TO A PERIODIC VARIATION

Energy Band Formation

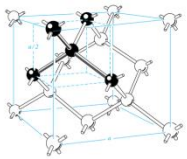


Energy Band Formation

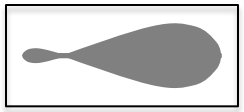


Gedanken Experiment

Imagine you start with $a \gg$ and then shrink down to exact size

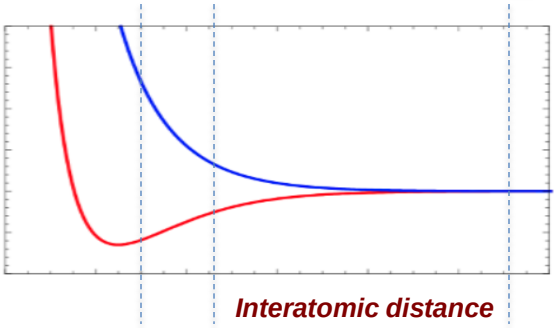


Stable crystal

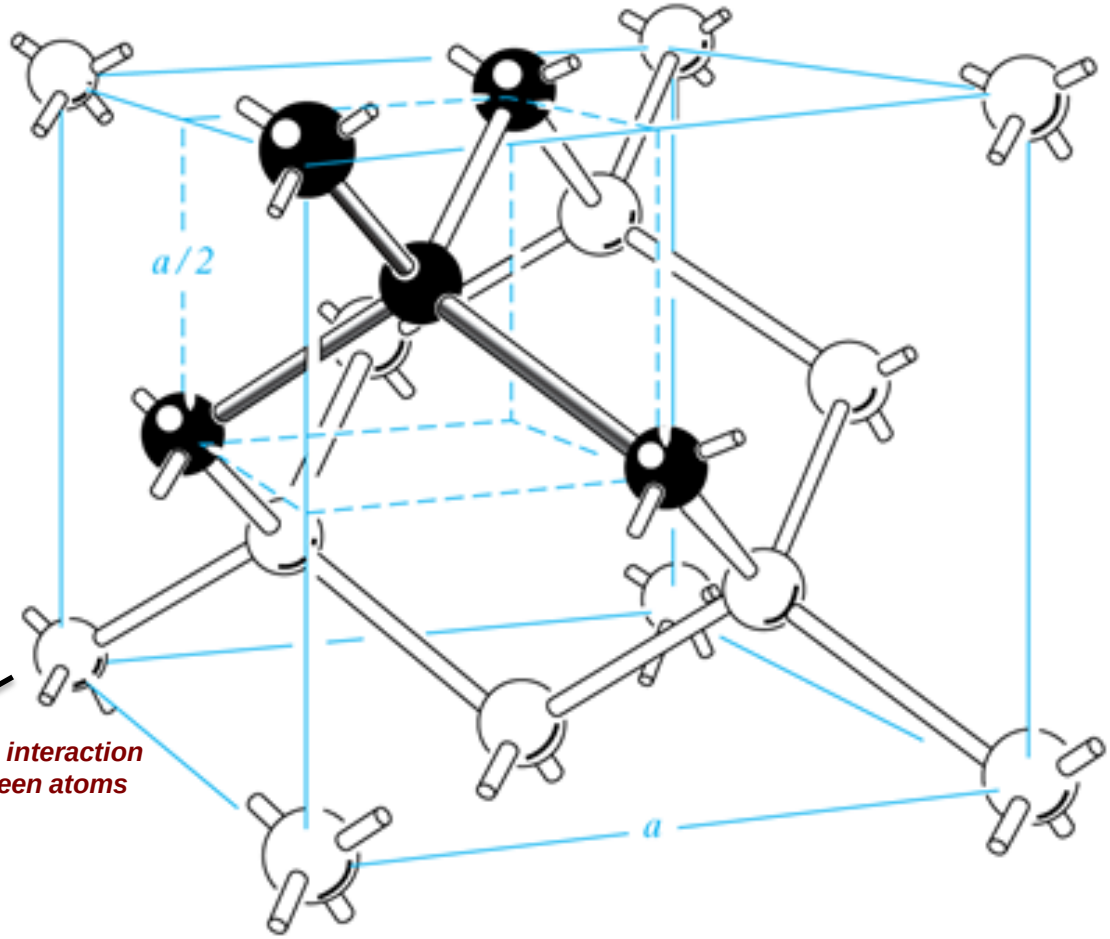


sp^3-Hybridization starts

Little interaction between atoms



Interatomic distance

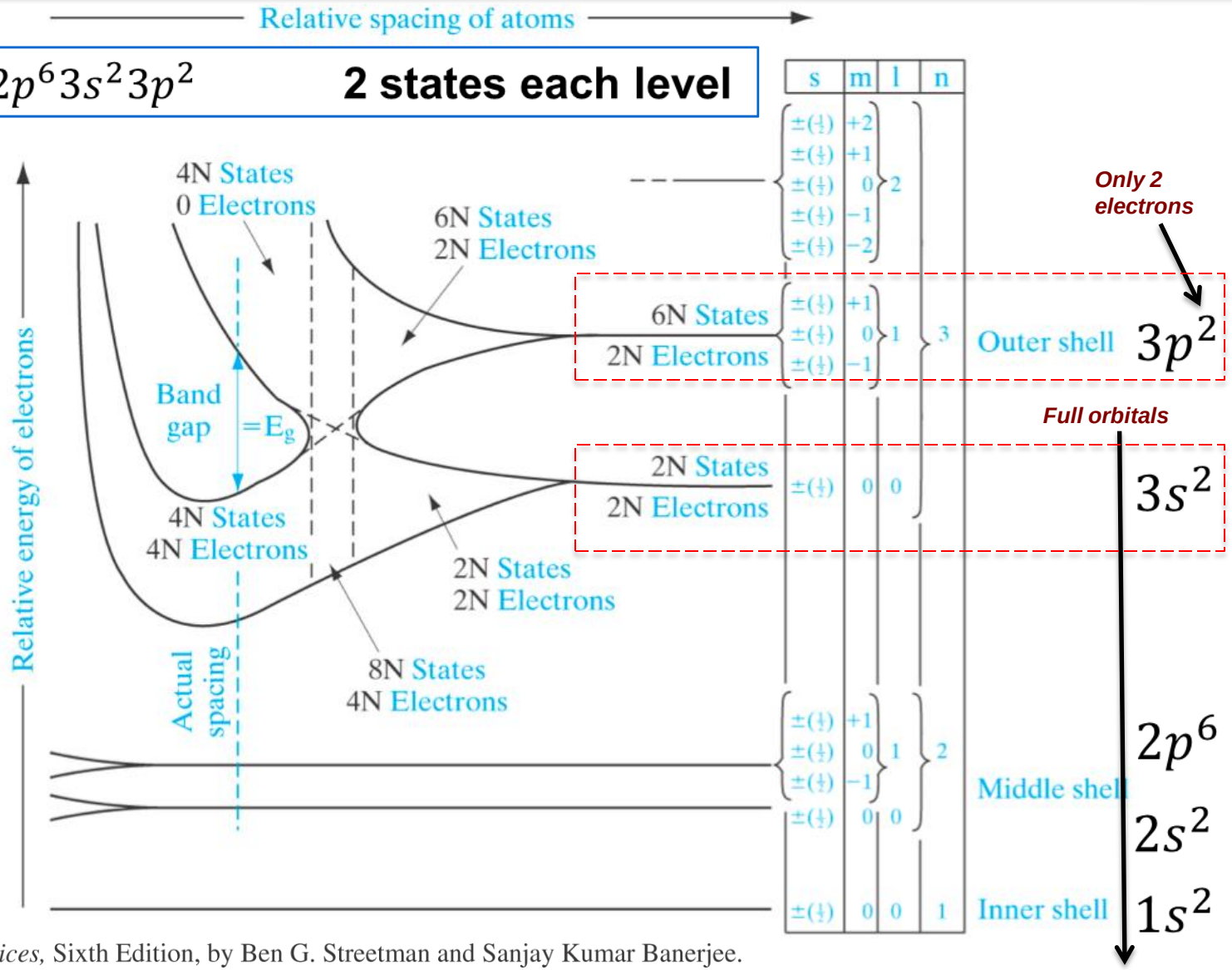


Energy Bands Formation

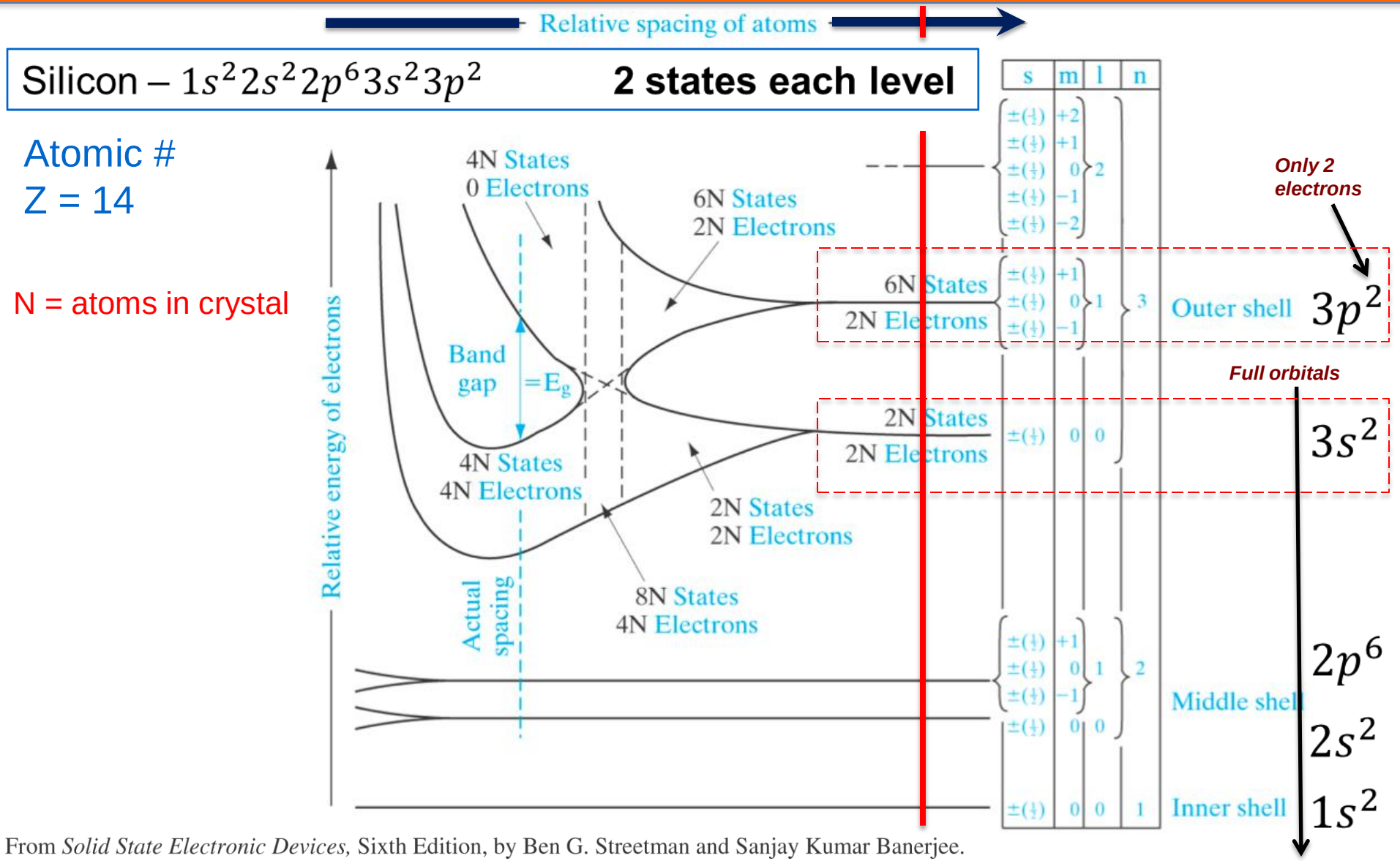
Silicon – $1s^2 2s^2 2p^6 3s^2 3p^2$ **2 states each level**

Atomic #
Z = 14

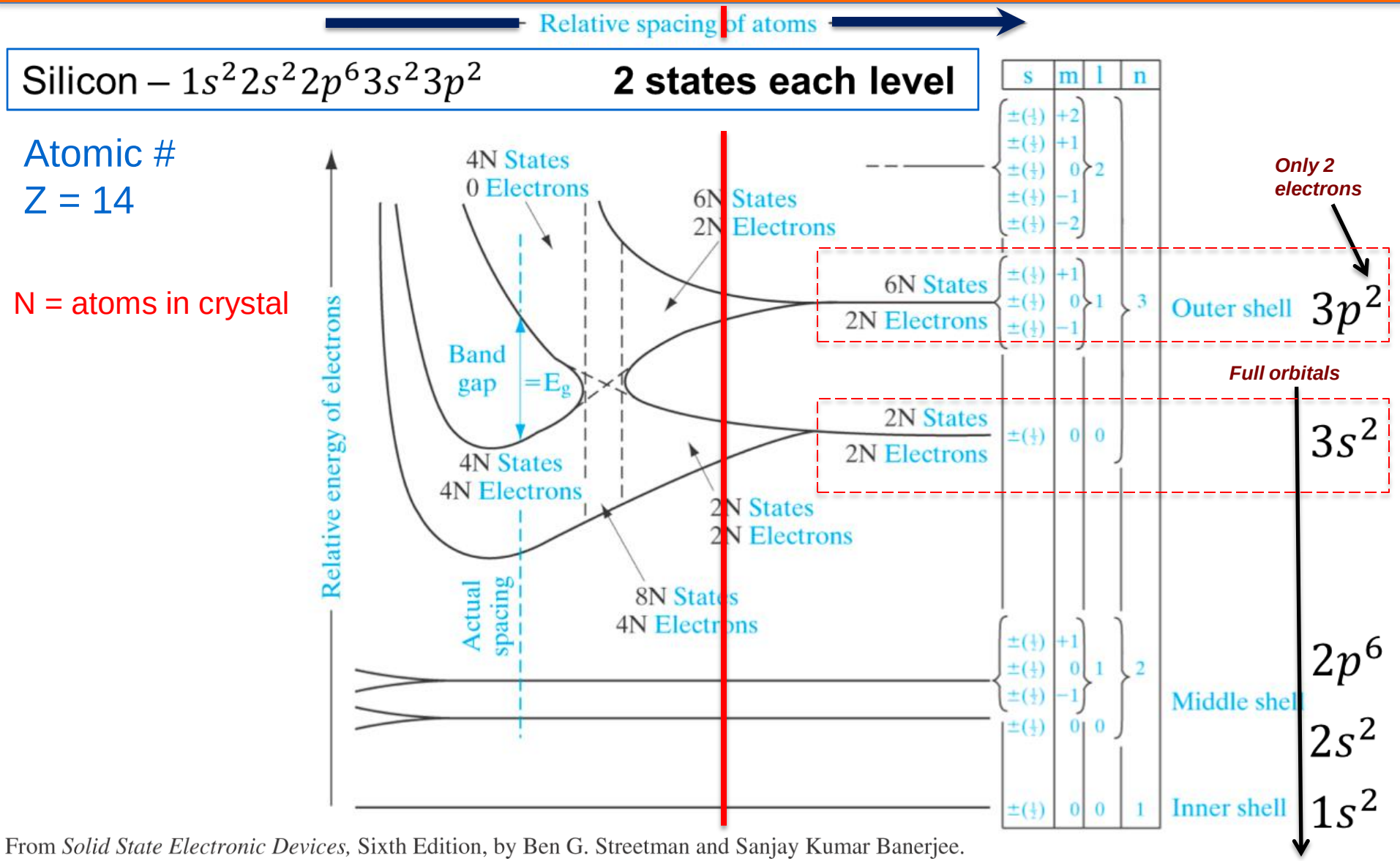
N = atoms in crystal



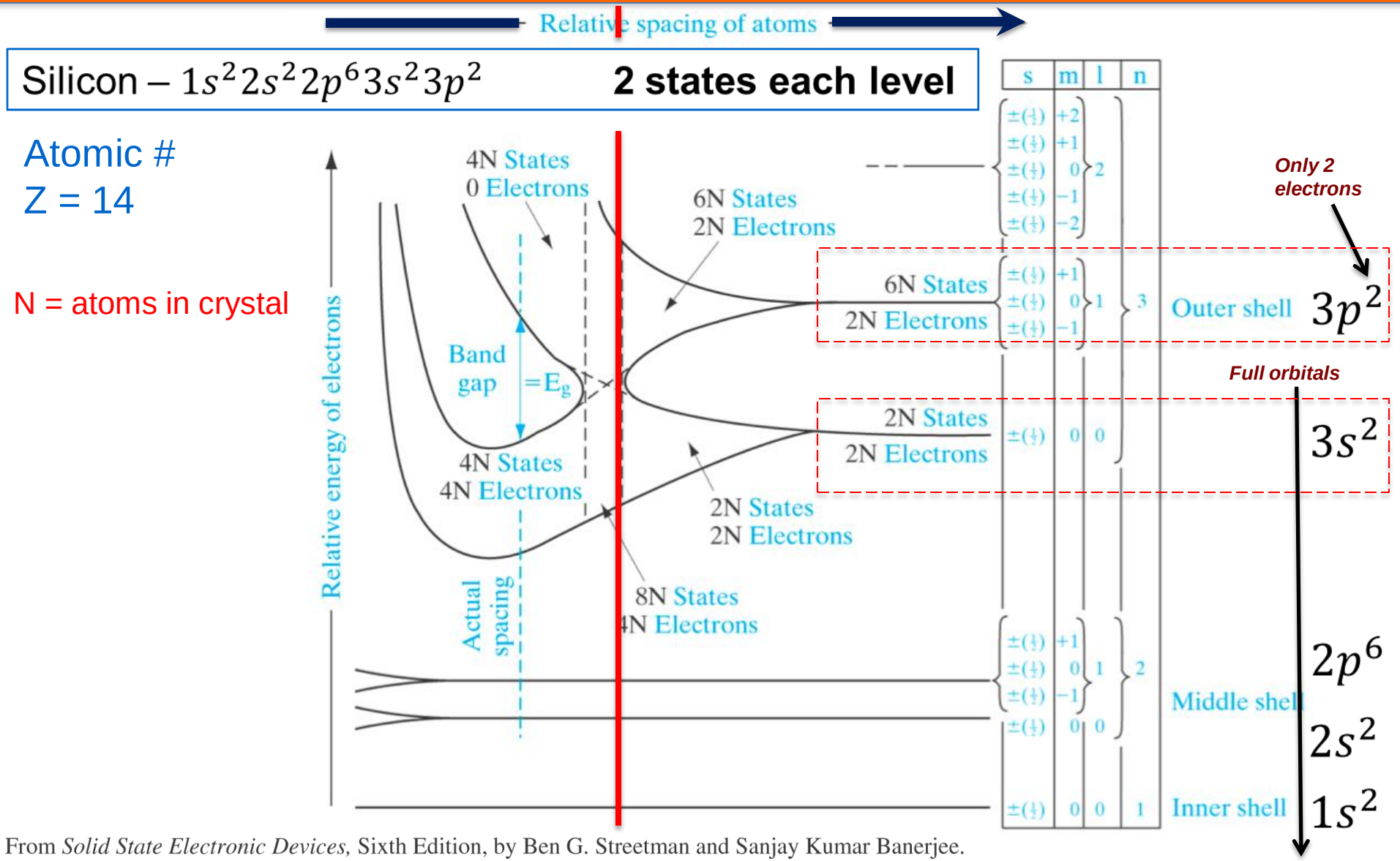
ATOMS ARE FAR AWAY FROM EACH OTHER AND DO NOT INTERACT



ATOMS START INTERACTING – BONDING & ANTIBONDING STATES START FORMING



STRONGER INTERACTION – sp^3 ORBITAL HYBRIDIZATION STARTS

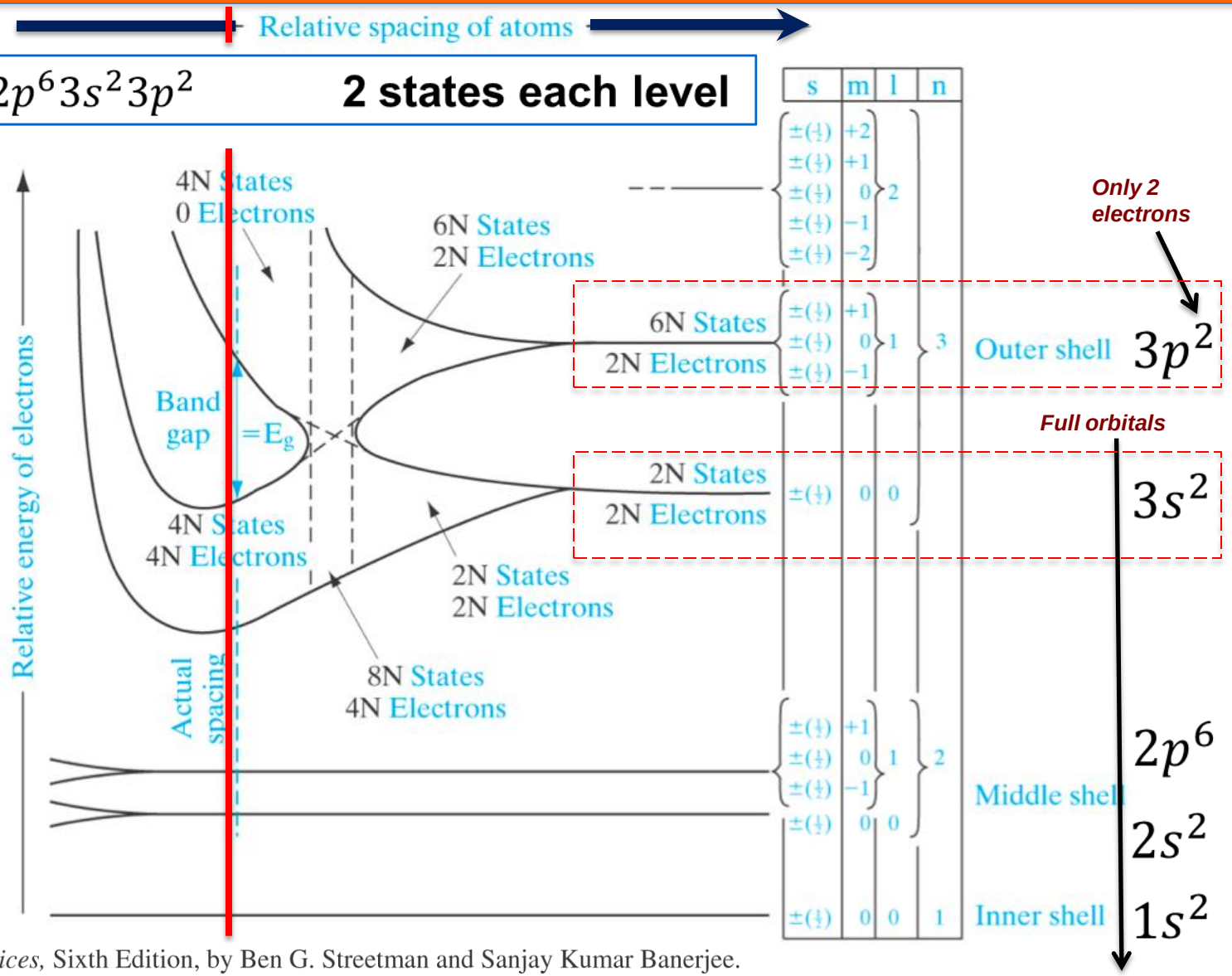


STABLE CRYSTAL CONFIGURATION REACHED – COVALENT BONDING VALENCE AND CONDUCTION BANDS WITH BAND GAP ARE FORMED

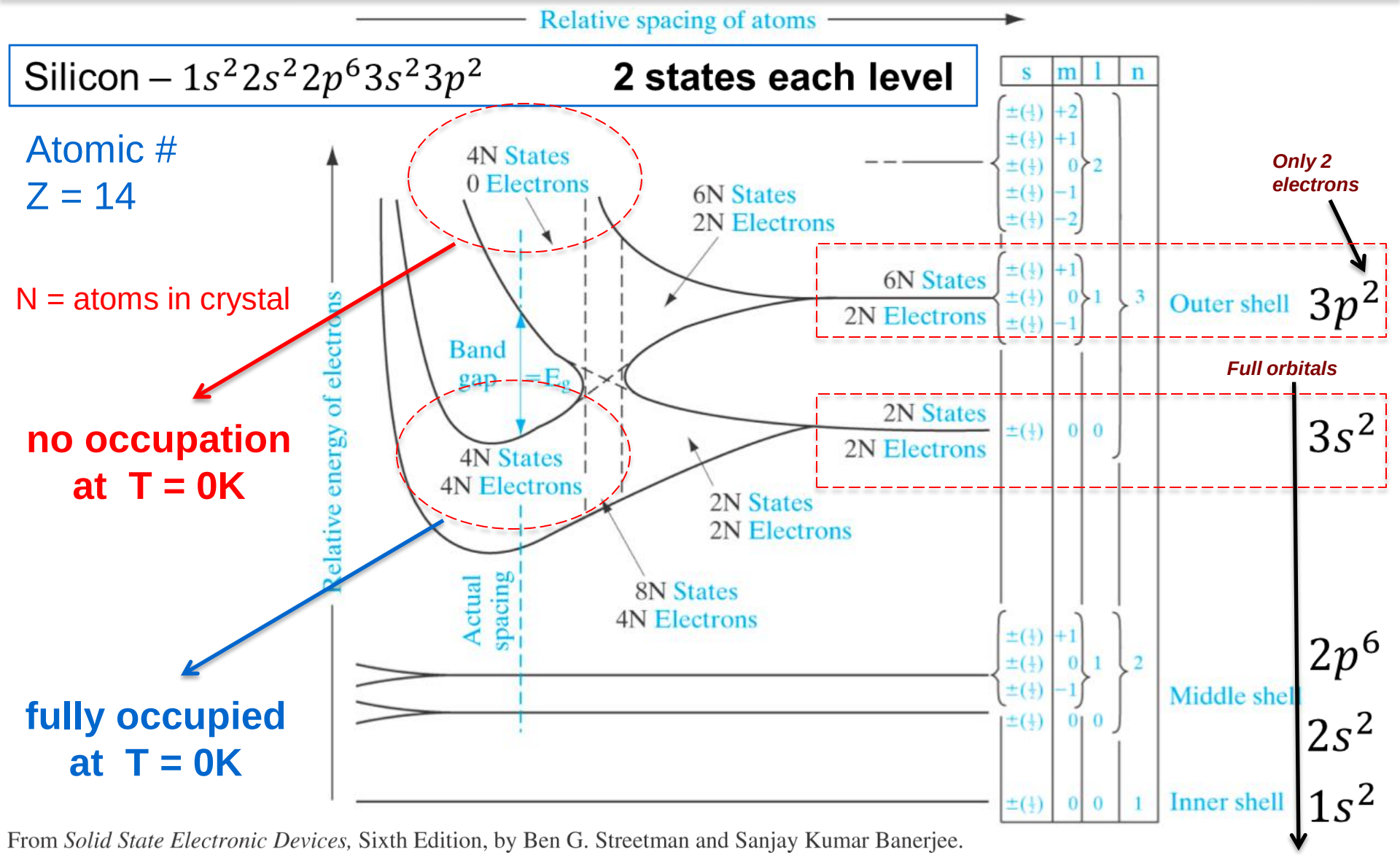
Silicon – $1s^2 2s^2 2p^6 3s^2 3p^2$ **2 states each level**

Atomic #
Z = 14

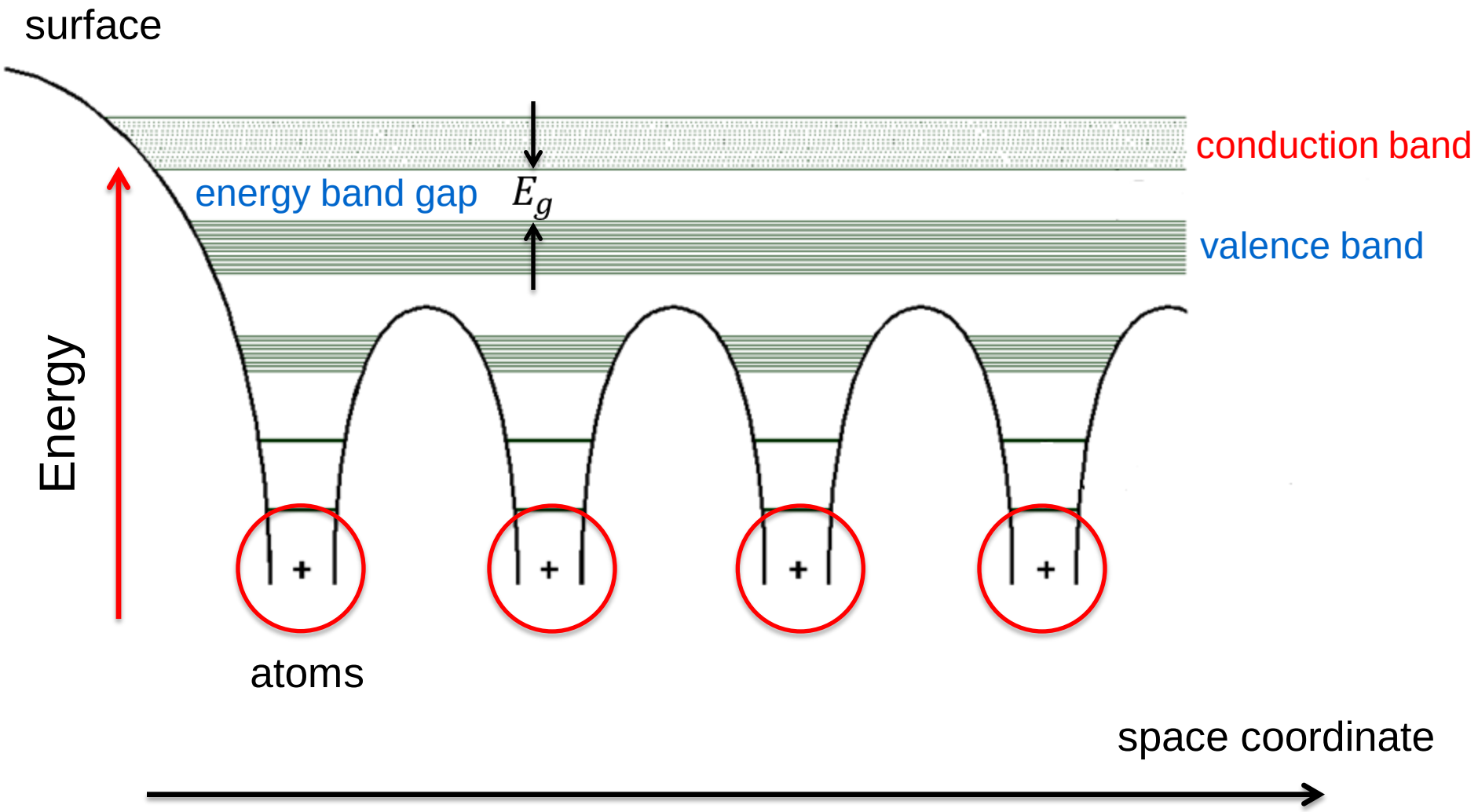
N = atoms in crystal



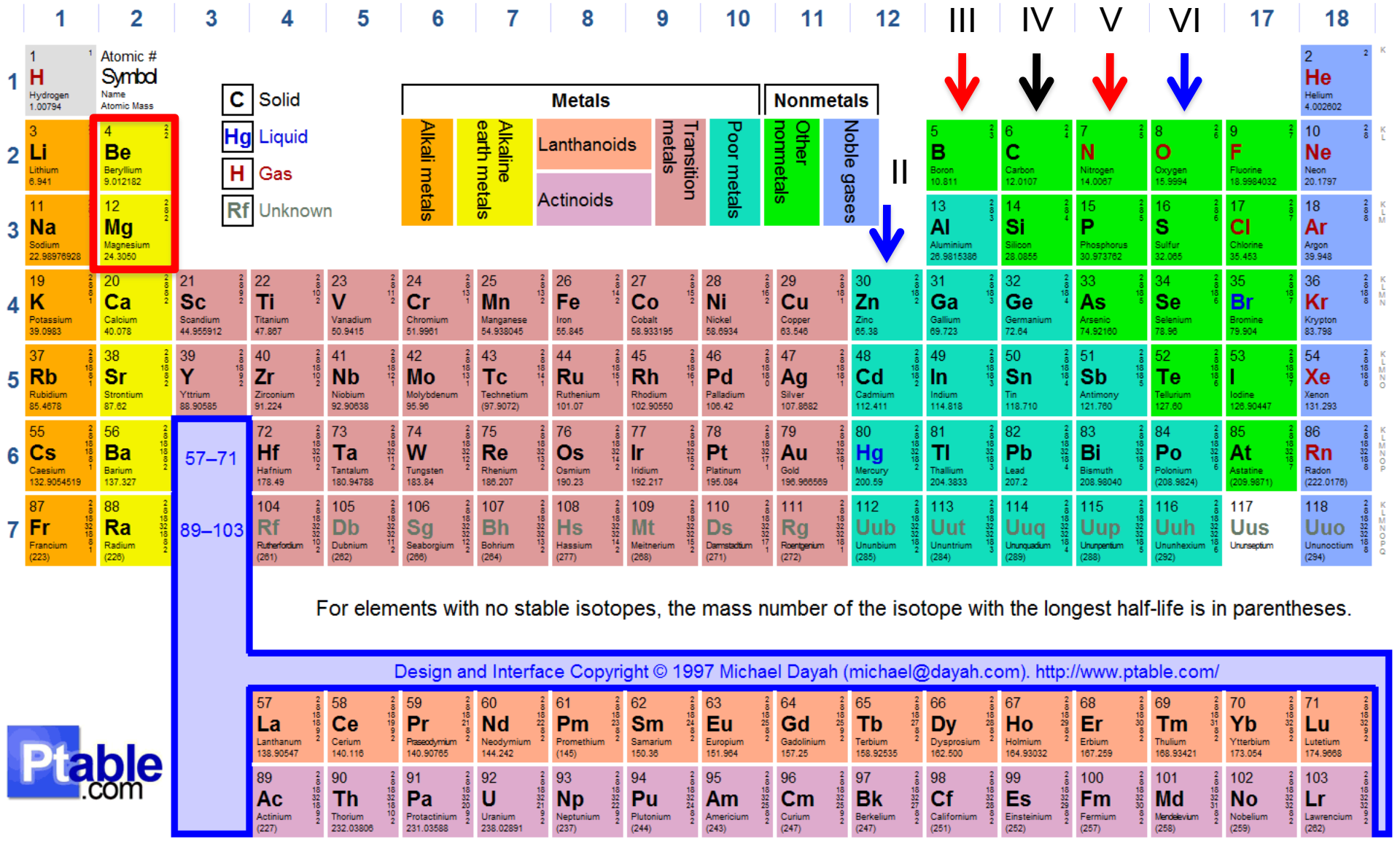
Energy Bands Formation



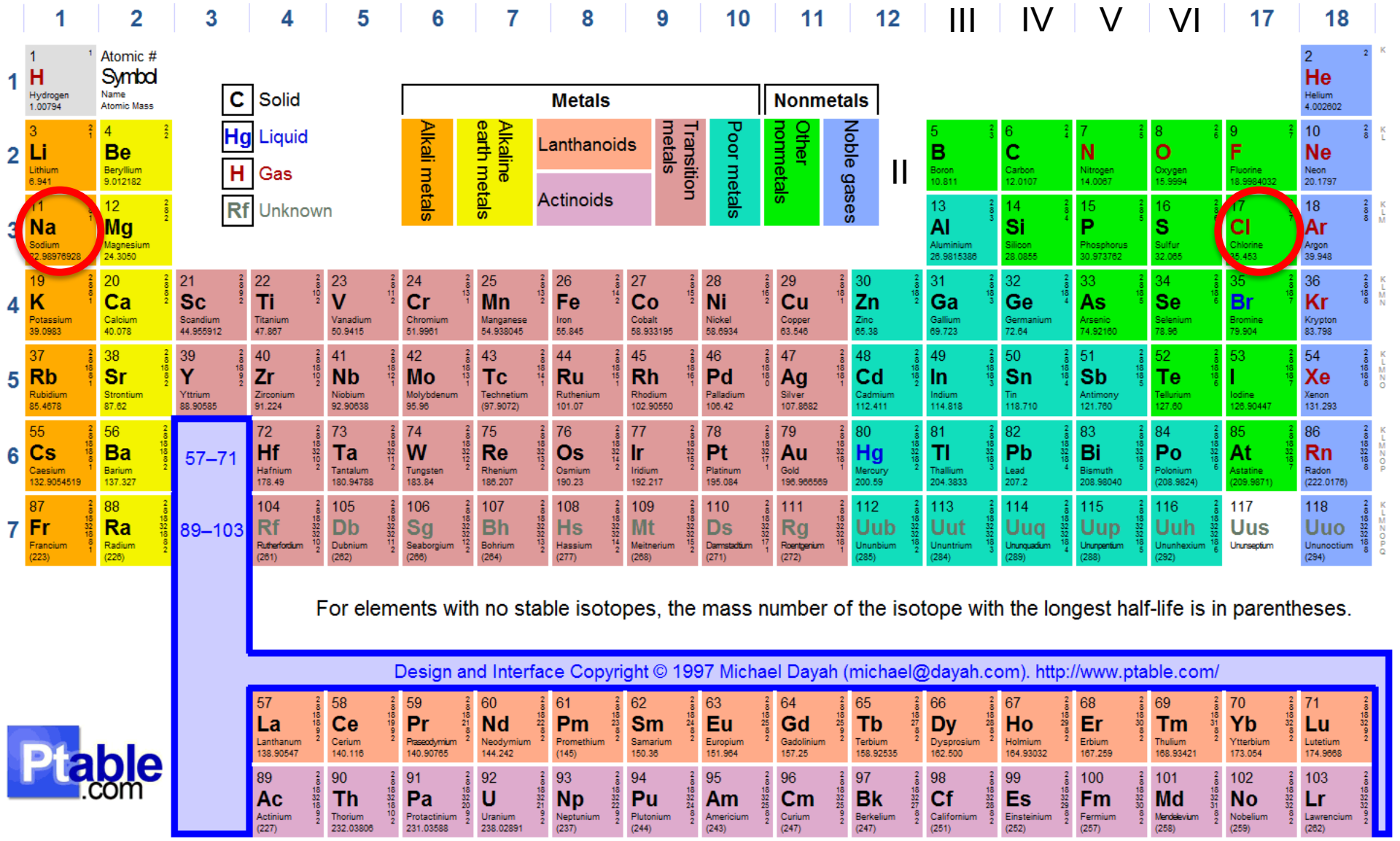
Energy Band Formation



Periodic Table of the Elements



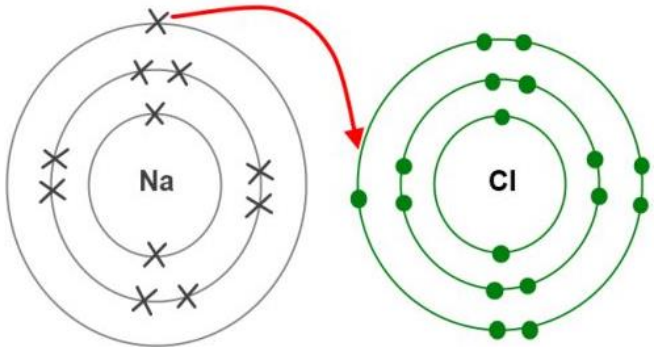
Ionic Bonding



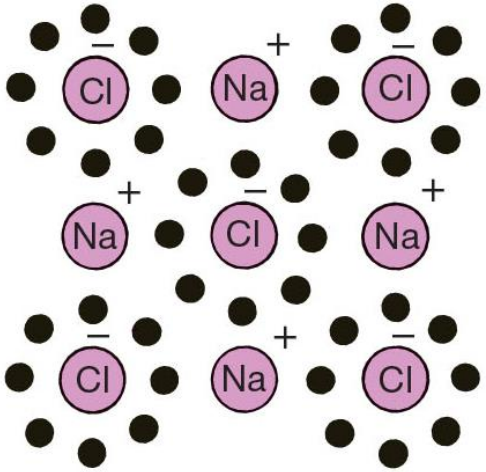
For elements with no stable isotopes, the mass number of the isotope with the longest half-life is in parentheses.

Ptable.com

Ionic Bonding

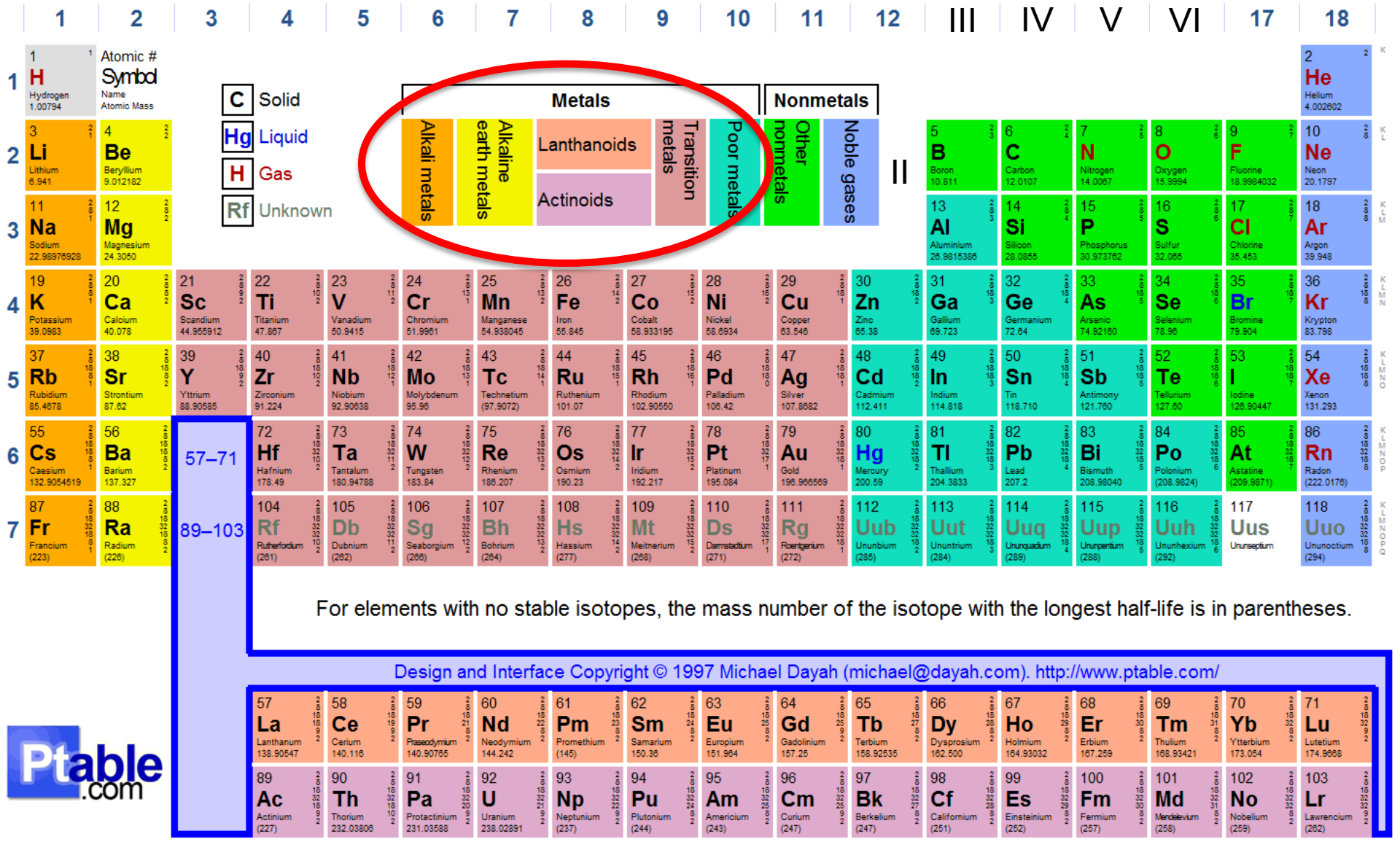


$= Na^+ \ \& \ Cl^-$

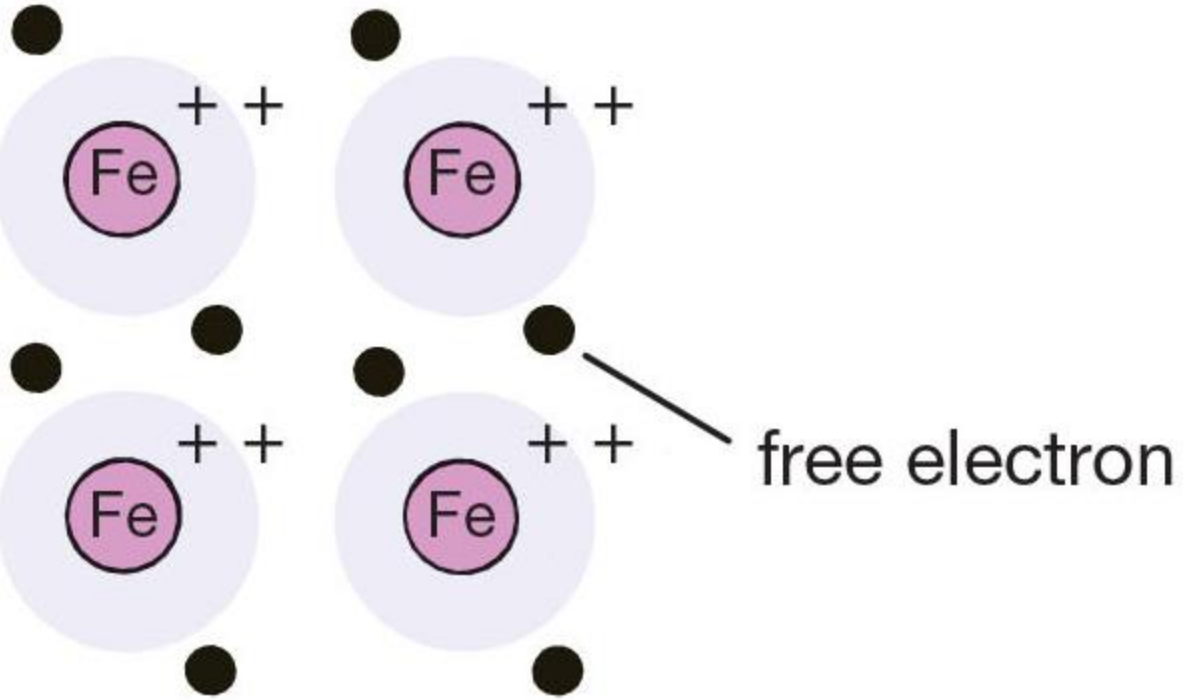


ionic bonding
electron transferred from Na to Cl

Metallic Bonding

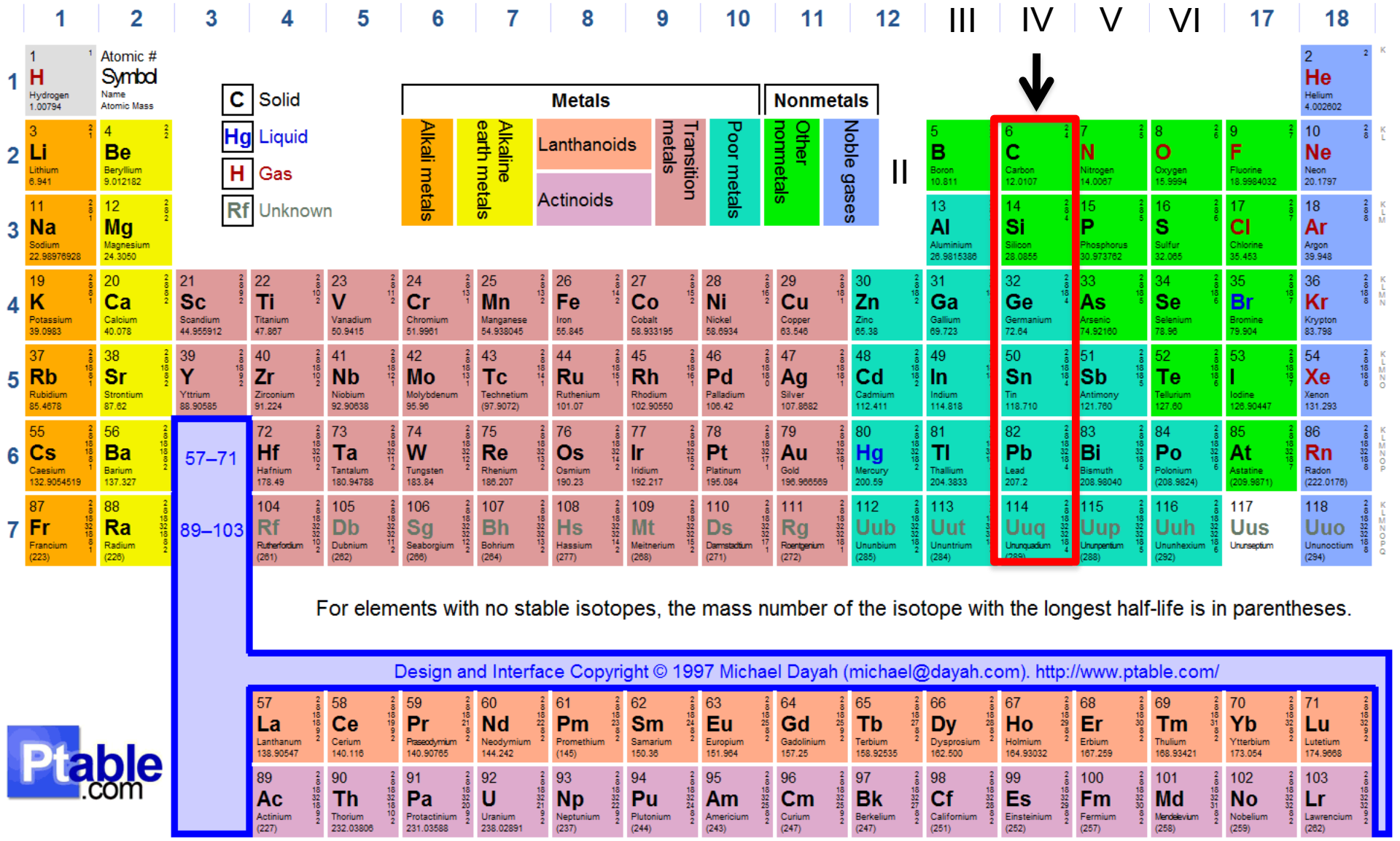


Metallic Bonding



metallic bonding
ions surrounded by free electrons

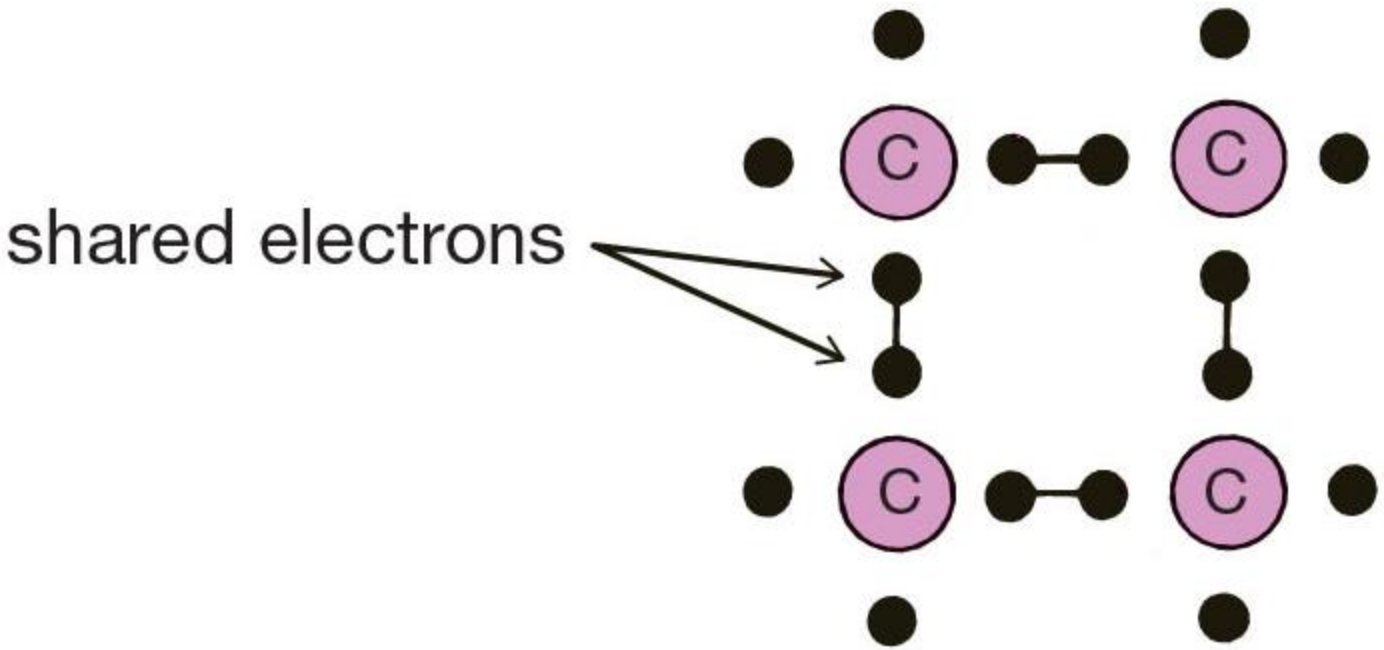
Covalent Bonding



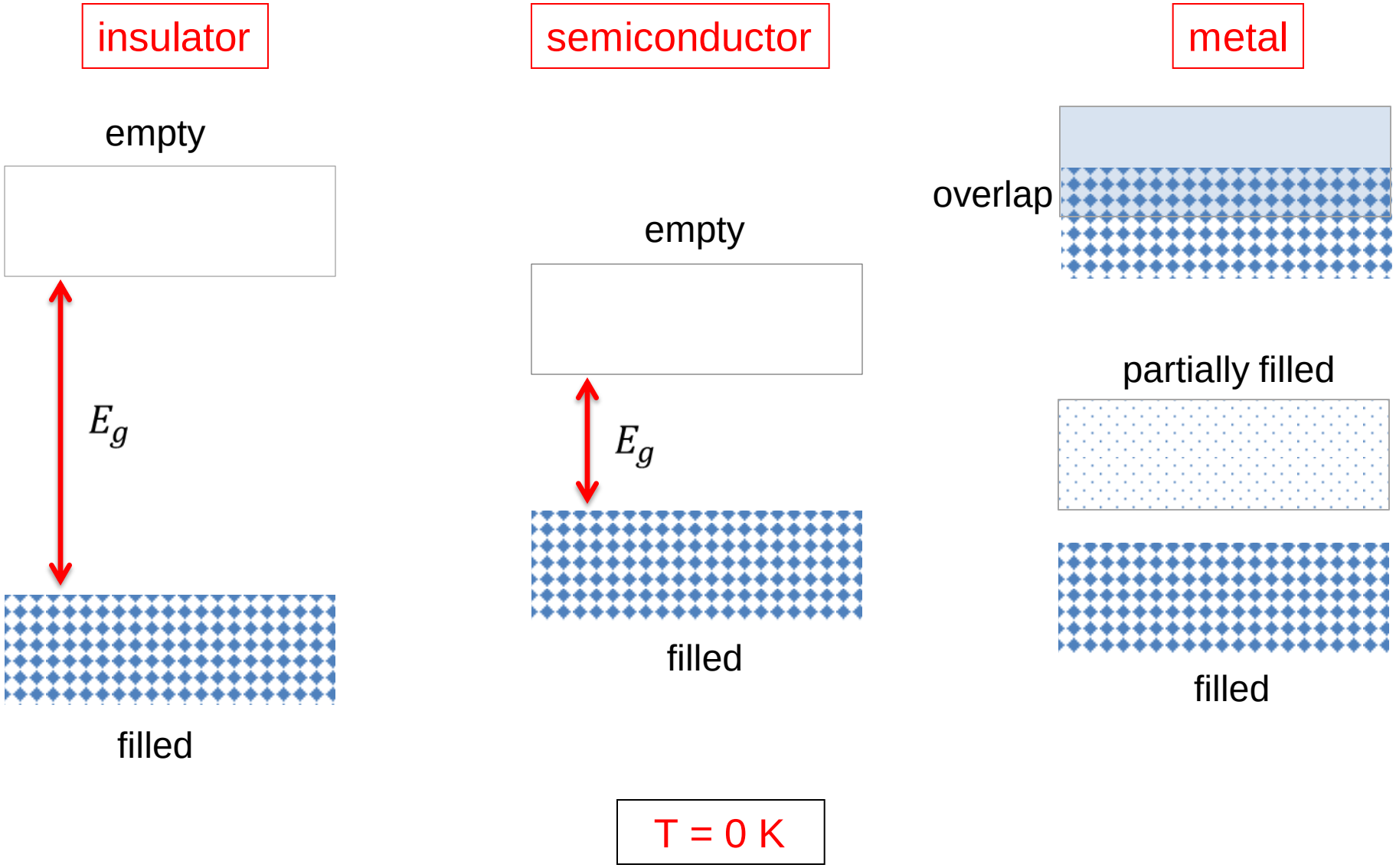
For elements with no stable isotopes, the mass number of the isotope with the longest half-life is in parentheses.

Ptable.com

Covalent Bonding



Behavioral Classification



Phase Space

Dynamics of electrons is studied in a generalized system of coordinates:

Time) t

Real Space) (x, y, z)

Momentum Space) (k_x, k_y, k_z)

} phase space

The kinetic energy state of the particle is given by a function

$$E = f(k_x, k_y, k_z)$$

This is usually known as “band structure”.
As we have seen, energy in a crystal is a multi-valued function, so the band structure has many branches.

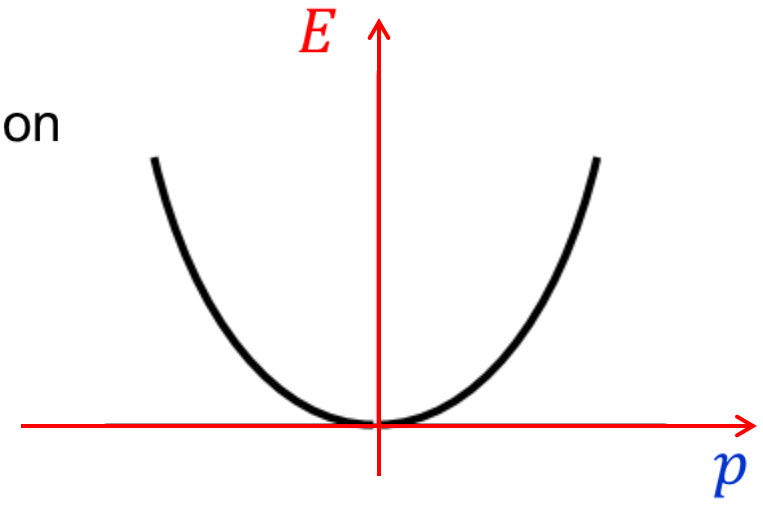
Classical particle

For a classical particle in free space there is only a single value of energy for each set of momentum coordinates.

$$E = \frac{1}{2}mv^2$$

Momentum is defined as $p = mv \rightarrow E = \frac{p^2}{2m}$

This is a simple parabolic relation



Quantum mechanical particle

For a quantum mechanical particle described by the Schrödinger equation inside a crystal, we define a new "crystal" momentum

$$\langle p \rangle = \hbar k$$

Here $\boldsymbol{k}$ is the wave number of the wave describing the particle quantum-mechanically and for convenience it is used most often as momentum coordinate.

Quantum mechanical particle

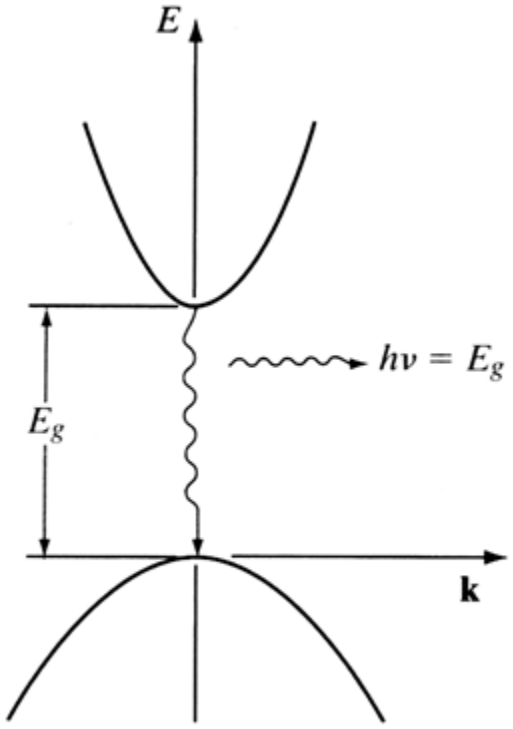
We model the crystal as a new kind of “free space” where the particles obey a new energy-momentum relationship given by the band structure, containing the effects of the periodic atomic potentials.

Therefore, what we study is not an electron “particle” as in an isolated atom or in vacuum, but an electron “quasi-particle” which obeys special dynamic laws as dictated by the specific crystal in which it moves.

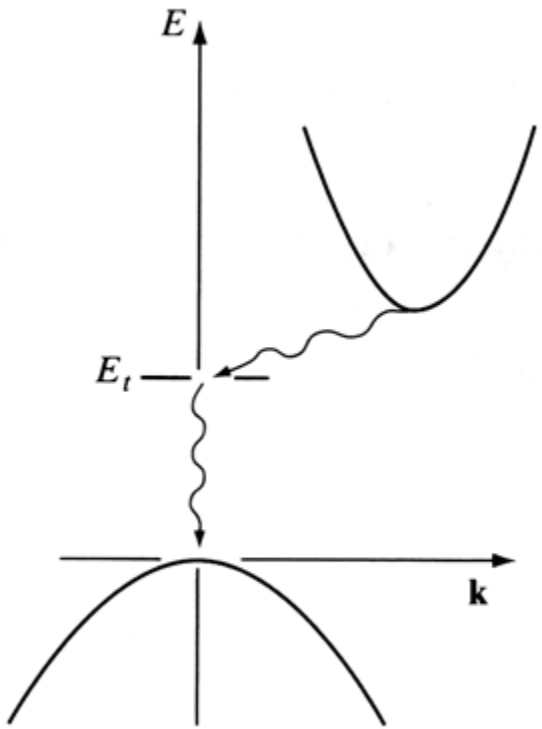
Simple examples of band structure

Lowest energy solution in the conduction band

Highest energy solution in the valence band



(a) Direct

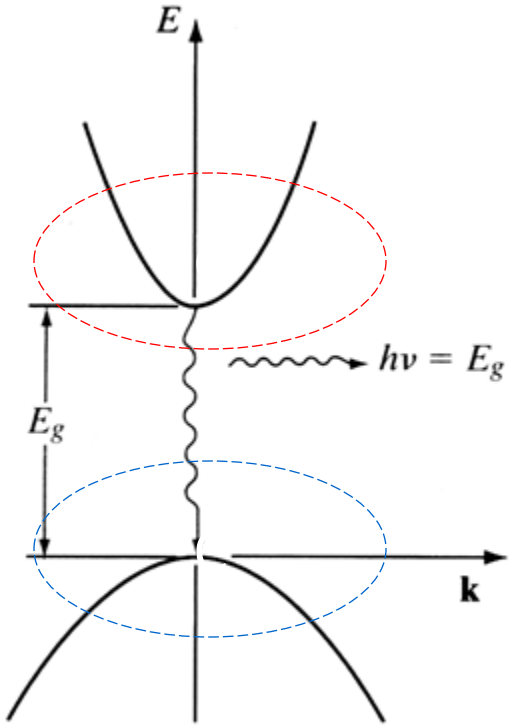


(b) Indirect

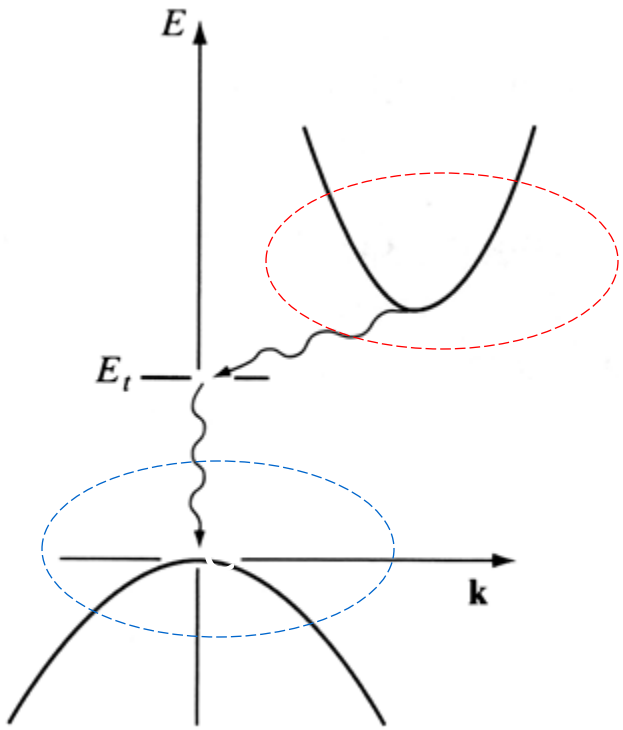
Simple examples of band structure

Often it is sufficient to analyze conduction band behavior only in the region close to the minimum of the lowest energy branch, called a “valley”.

In many cases the E(k) relations in the valleys are with good approximation parabolic



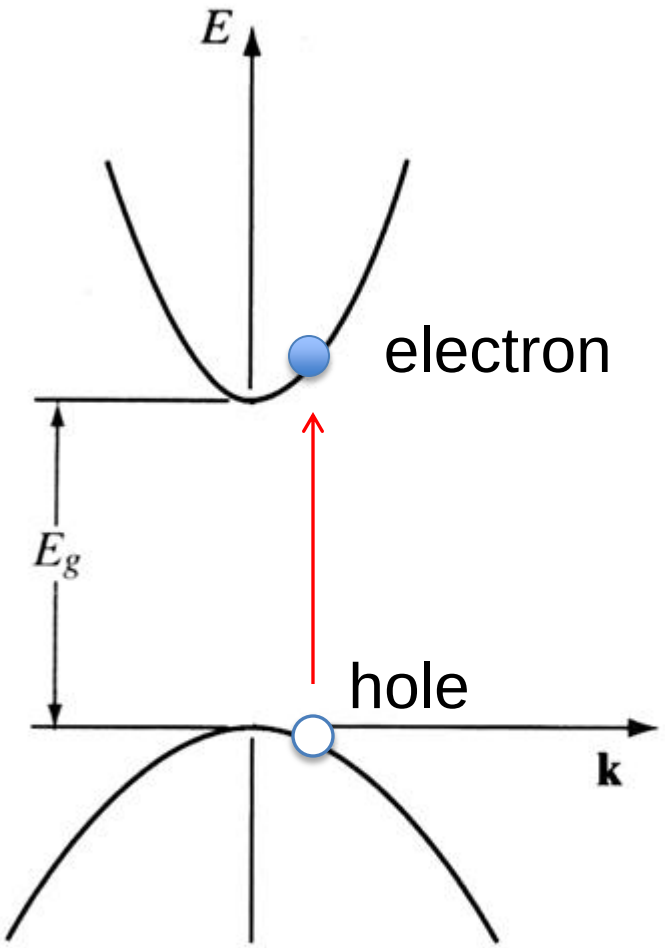
(a) Direct



(b) Indirect

Often it is sufficient to analyze valence band behavior only in the region close to the maximum of the highest energy branch, also called a “valley”.

Simple examples of band structure

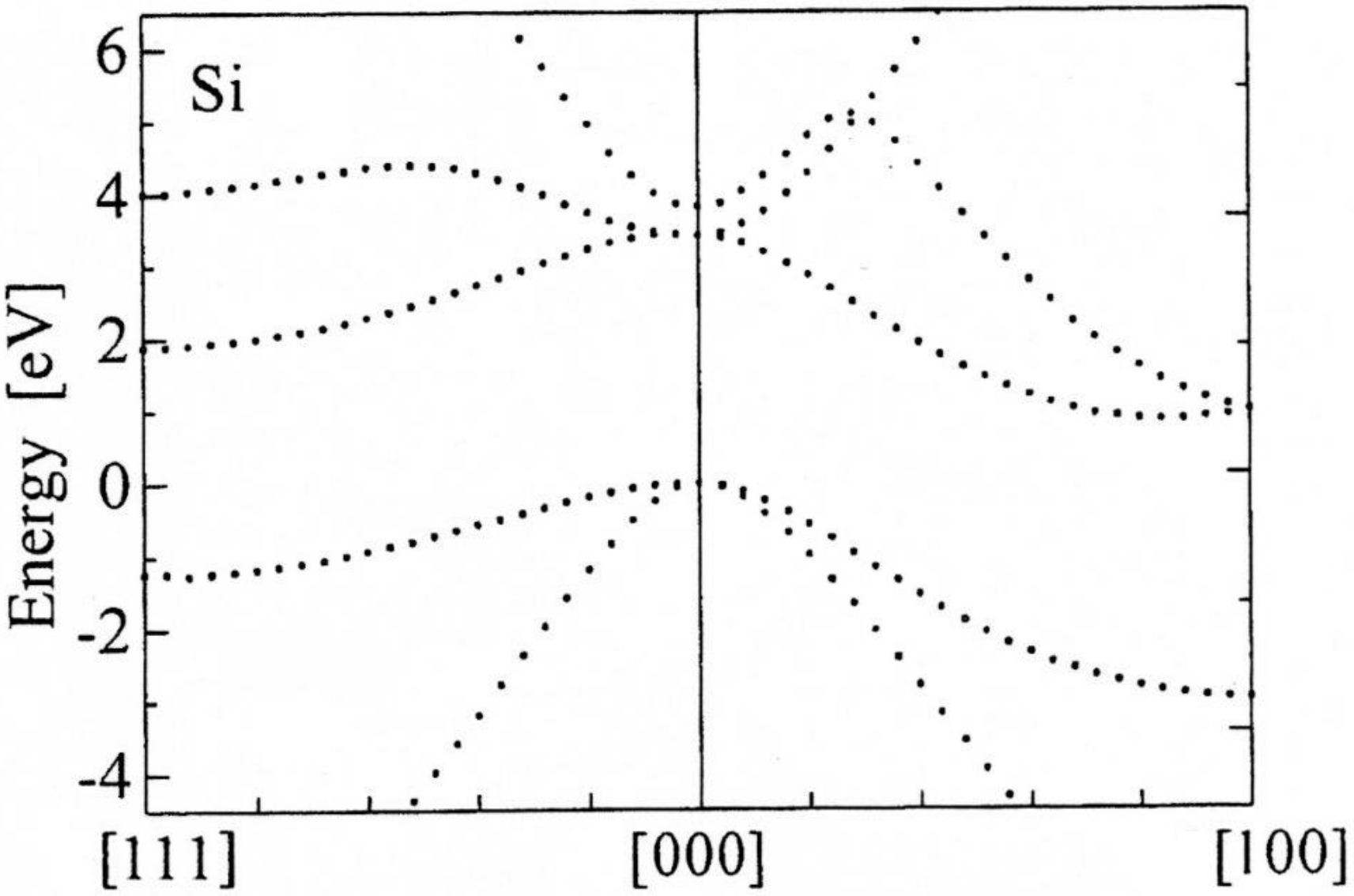


(a) Direct

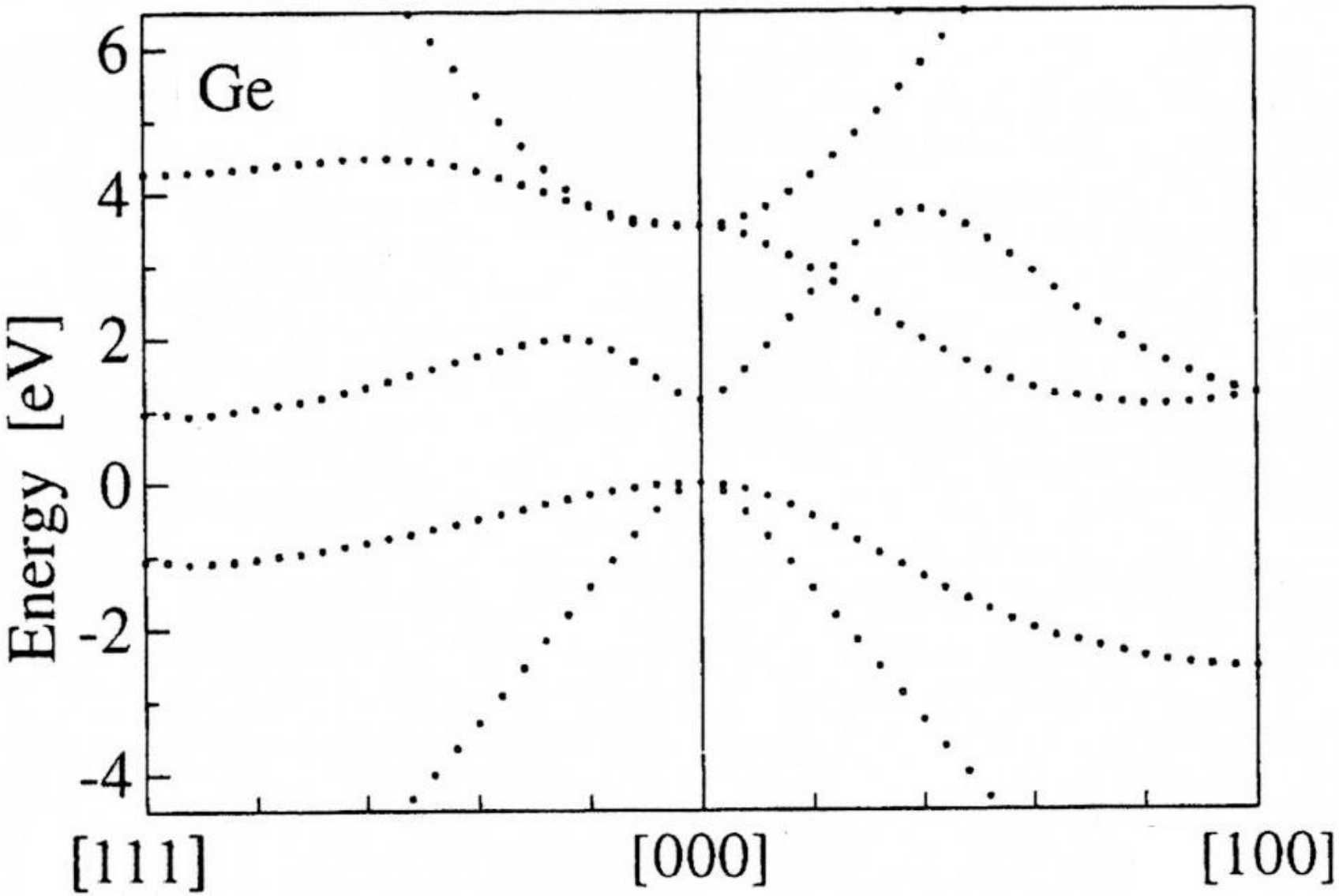
At finite temperature, electrons have the probability to acquire sufficient thermal energy to be excited to the conduction band.

An empty state is left behind, which essentially behaves like a positive "quasi-particle" (hole) moving when neighboring valence electron jump into that empty space leaving another one behind

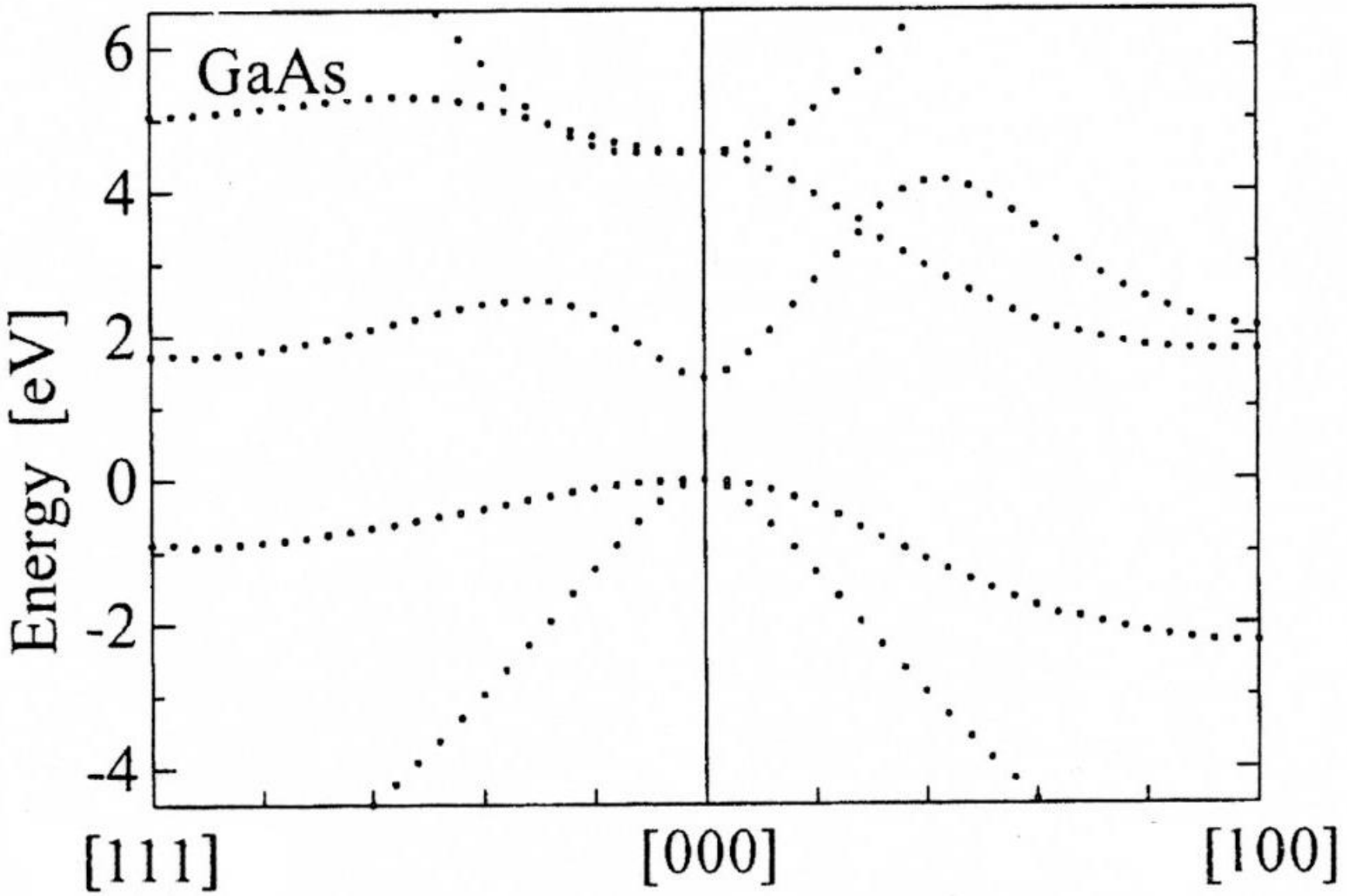
Direct or indirect?



Direct or indirect?



Direct or indirect?



Semiconductor Material Properties

		E_g (eV)	μ_n (cm^2/V-s)	μ_p (cm^2/V-s)	m^*_n/m_o (m_l, m_t)	m^*_p/m_o (m_{lh}, m_{hh})	a (Å)	ϵ_r	Density (g/cm^3)	Melting point (°C)
Si	(*i/D*)	1.11	1350	480	0.98, 0.19	0.16, 0.49	5.43	11.8	2.33	1415
Ge	(*i/D*)	0.67	3900	1900	1.64, 0.082	0.04, 0.28	5.65	16	5.32	936
SiC (α)	(*i/W*)	2.86	500	—	0.6	1.0	3.08	10.2	3.21	2830
AlP	(*i/Z*)	2.45	80	—	—	0.2, 0.63	5.46	9.8	2.40	2000
AlAs	(*i/Z*)	2.16	1200	420	2.0	0.15, 0.76	5.66	10.9	3.60	1740
AlSb	(*i/Z*)	1.6	200	300	0.12	0.98	6.14	11	4.26	1080
GaP	(*i/Z*)	2.26	300	150	1.12, 0.22	0.14, 0.79	5.45	11.1	4.13	1467
GaAs	(*d/Z*)	1.43	8500	400	0.067	0.074, 0.50	5.65	13.2	5.31	1238
GaN	(*d/Z, W*)	3.4	380	—	0.19	0.60	4.5	12.2	6.1	2530
GaSb	(*d/Z*)	0.7	5000	1000	0.042	0.06, 0.23	6.09	15.7	5.61	712
InP	(*d/Z*)	1.35	4000	100	0.077	0.089, 0.85	5.87	12.4	4.79	1070
InAs	(*d/Z*)	0.36	22600	200	0.023	0.025, 0.41	6.06	14.6	5.67	943
InSb	(*d/Z*)	0.18	10^5	1700	0.014	0.015, 0.40	6.48	17.7	5.78	525
ZnS	(*d/Z, W*)	3.6	180	10	0.28	—	5.409	8.9	4.09	1650*
ZnSe	(*d/Z*)	2.7	600	28	0.14	0.60	5.671	9.2	5.65	1100*
ZnTe	(*d/Z*)	2.25	530	100	0.18	0.65	6.101	10.4	5.51	1238*
CdS	(*d/W, Z*)	2.42	250	15	0.21	0.80	4.137	8.9	4.82	1475
CdSe	(*d/W*)	1.73	800	—	0.13	0.45	4.30	10.2	5.81	1258
CdTe	(*d/Z*)	1.58	1050	100	0.10	0.37	6.482	10.2	6.20	1098
PbS	(*i/H*)	0.37	575	200	0.22	0.29	5.936	17.0	7.6	1119
PbSe	(*i/H*)	0.27	1500	1500	—	—	6.147	23.6	8.73	1081
PbTe	(*i/H*)	0.29	6000	4000	0.17	0.20	6.452	30	8.16	925

All values at 300 K.

*Vaporizes

C (diamond)
$E_g = 5.5eV$

SiO_2
$E_g = 9.0eV$