

Applying MO theory to other systems

**Conducting materials (metals/semiconductors)
show similar behaviour**

Metallic Properties

Metallic Character decreases

Metallic character increases

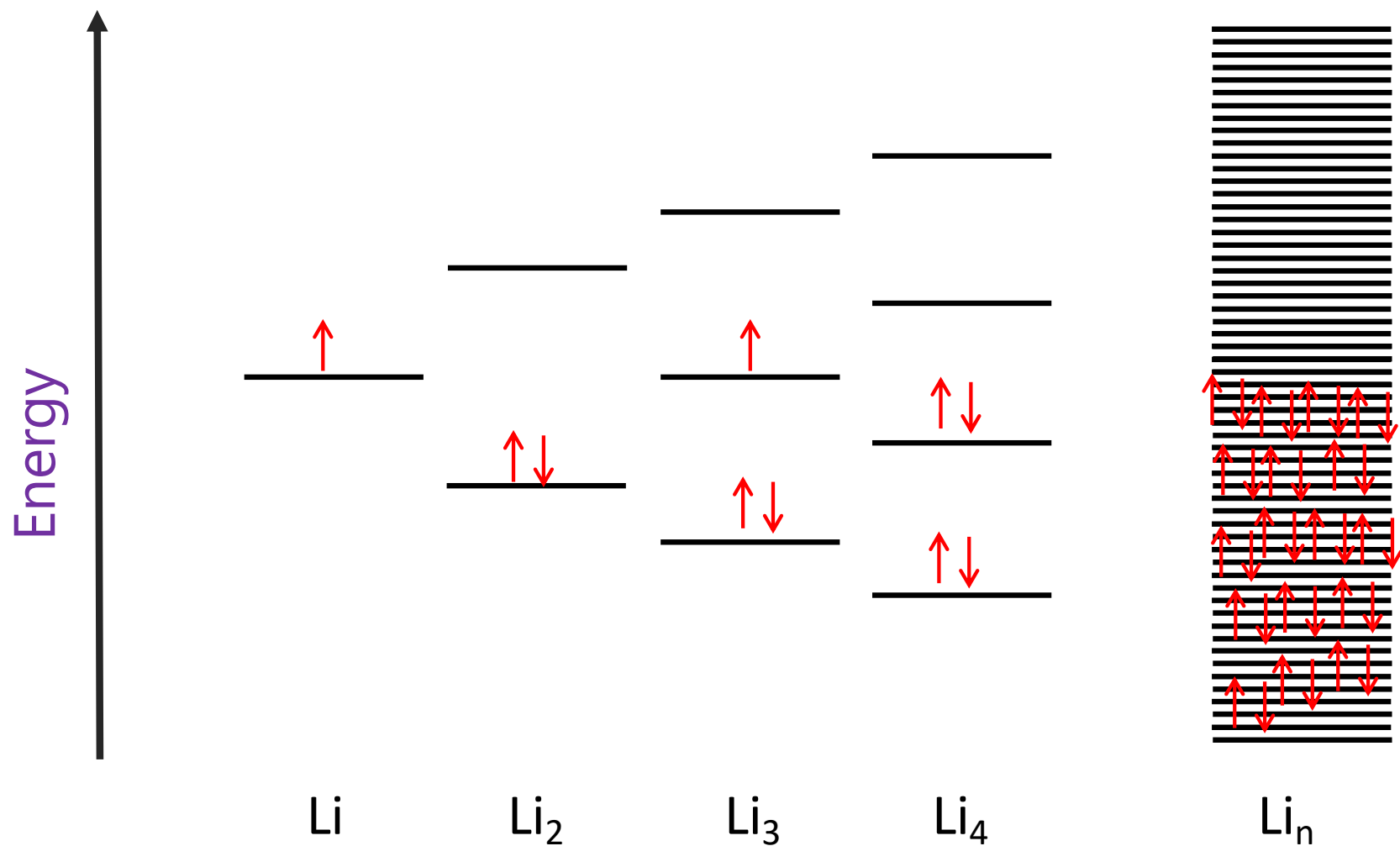
Main-Group Elements (s block)		Transition Elements (d block)										Main-Group Elements (p block)					
1																	
ns ¹																	
1	2											13	14	15	16	17	18
1s ¹	ns ²											ns ² np ¹	ns ² np ²	ns ² np ³	ns ² np ⁴	ns ² np ⁵	ns ² np ⁶
1	2											5	6	7	8	9	10
H	He											B	C	N	O	F	Ne
1s ¹	1s ²											2s ² 2p ¹	2s ² 2p ²	2s ² 2p ³	2s ² 2p ⁴	2s ² 2p ⁵	2s ² 2p ⁶
2	2											13	14	15	16	17	18
Li	Be											Al	Si	P	S	Cl	Ar
2s ¹	2s ²											3s ² 3p ¹	3s ² 3p ²	3s ² 3p ³	3s ² 3p ⁴	3s ² 3p ⁵	3s ² 3p ⁶
3	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
Na	Mg	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
3s ¹	3s ²	4s ² 3d ¹	4s ² 3d ²	4s ² 3d ³	4s ¹ 3d ⁵	4s ² 3d ⁵	4s ² 3d ⁶	4s ² 3d ⁷	4s ² 3d ⁸	4s ¹ 3d ¹⁰	4s ² 3d ¹⁰	4s ² 4p ¹	4s ² 4p ²	4s ² 4p ³	4s ² 4p ⁴	4s ² 4p ⁵	4s ² 4p ⁶
4	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
4s ¹	4s ²	4s ² 3d ¹	4s ² 3d ²	4s ² 3d ³	4s ¹ 3d ⁵	4s ² 3d ⁵	4s ² 3d ⁶	4s ² 3d ⁷	4s ² 3d ⁸	4s ¹ 3d ¹⁰	4s ² 3d ¹⁰	4s ² 4p ¹	4s ² 4p ²	4s ² 4p ³	4s ² 4p ⁴	4s ² 4p ⁵	4s ² 4p ⁶
5	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
5s ¹	5s ²	5s ² 4d ¹	5s ² 4d ²	5s ¹ 4d ⁴	5s ² 4d ⁵	5s ² 4d ⁵	5s ¹ 4d ⁷	5s ² 4d ⁷	5s ¹ 4d ¹⁰	5s ² 4d ¹⁰	5s ² 4d ¹⁰	5s ² 5p ¹	5s ² 5p ²	5s ² 5p ³	5s ² 5p ⁴	5s ² 5p ⁵	5s ² 5p ⁶
6	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
Cs	Ba		Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
6s ¹	6s ²		6s ² 5d ²	6s ² 5d ³	6s ² 5d ⁴	6s ² 5d ⁵	6s ² 5d ⁶	6s ² 5d ⁷	6s ¹ 5d ⁹	6s ¹ 5d ¹⁰	6s ² 5d ¹⁰	6s ² 6p ¹	6s ² 6p ²	6s ² 6p ³	6s ² 6p ⁴	6s ² 6p ⁵	6s ² 6p ⁶
7	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
Fr	Ra		Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Uut	Fl	Uup	Lv	Uus	Uuo
7s ¹	7s ²		7s ² 6d ²	7s ² 6d ³	7s ² 6d ⁴	7s ² 6d ⁵	7s ² 6d ⁶	7s ² 6d ⁷	7s ² 6d ⁸	7s ² 6d ⁹	7s ² 6d ¹⁰	7s ² 7p ¹	7s ² 7p ²	7s ² 7p ³	7s ² 7p ⁴	7s ² 7p ⁵	7s ² 7p ⁶

Metals

- Shiny solids
- Moderate to high melting point
- Good conductors: heat & electricity
- Lose electrons to nonmetals

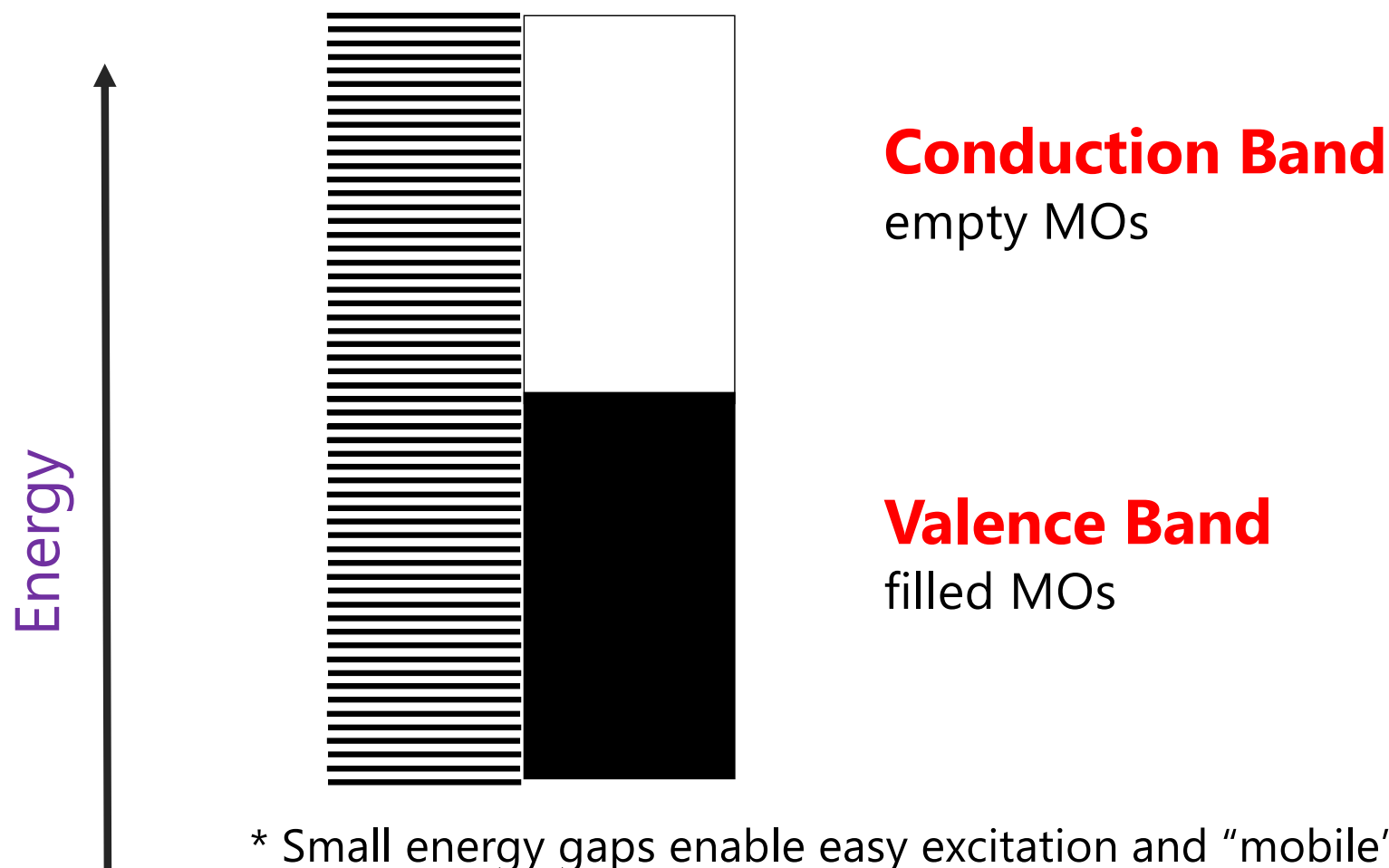
Band Theory: Group 1 Metals

Li_n (metal): n 2s AOs = n MOs (n valence electrons)



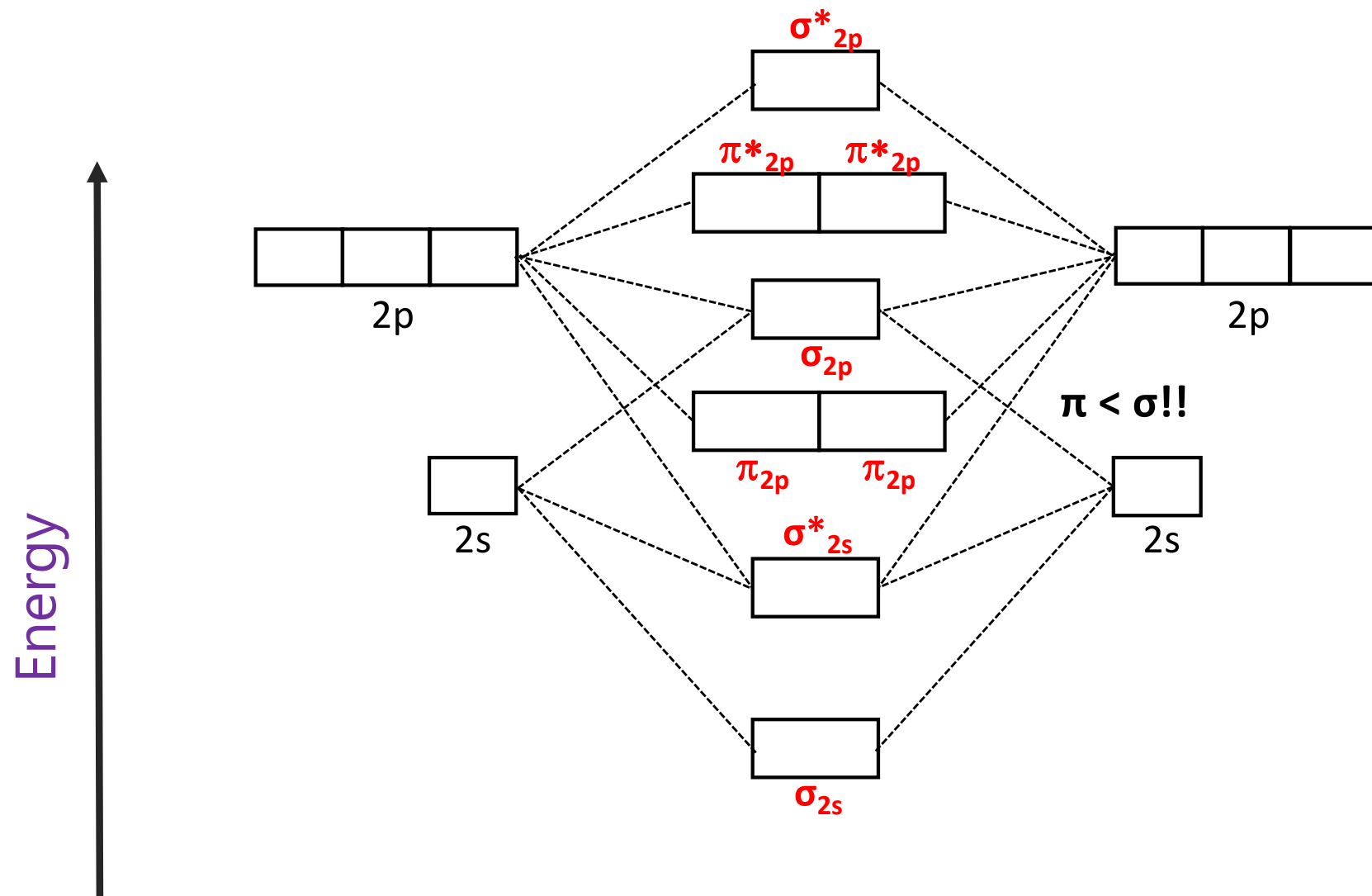
Li 2s Energy Band

Li_n (metal): n 2s AOs = n MOs (n valence electrons)



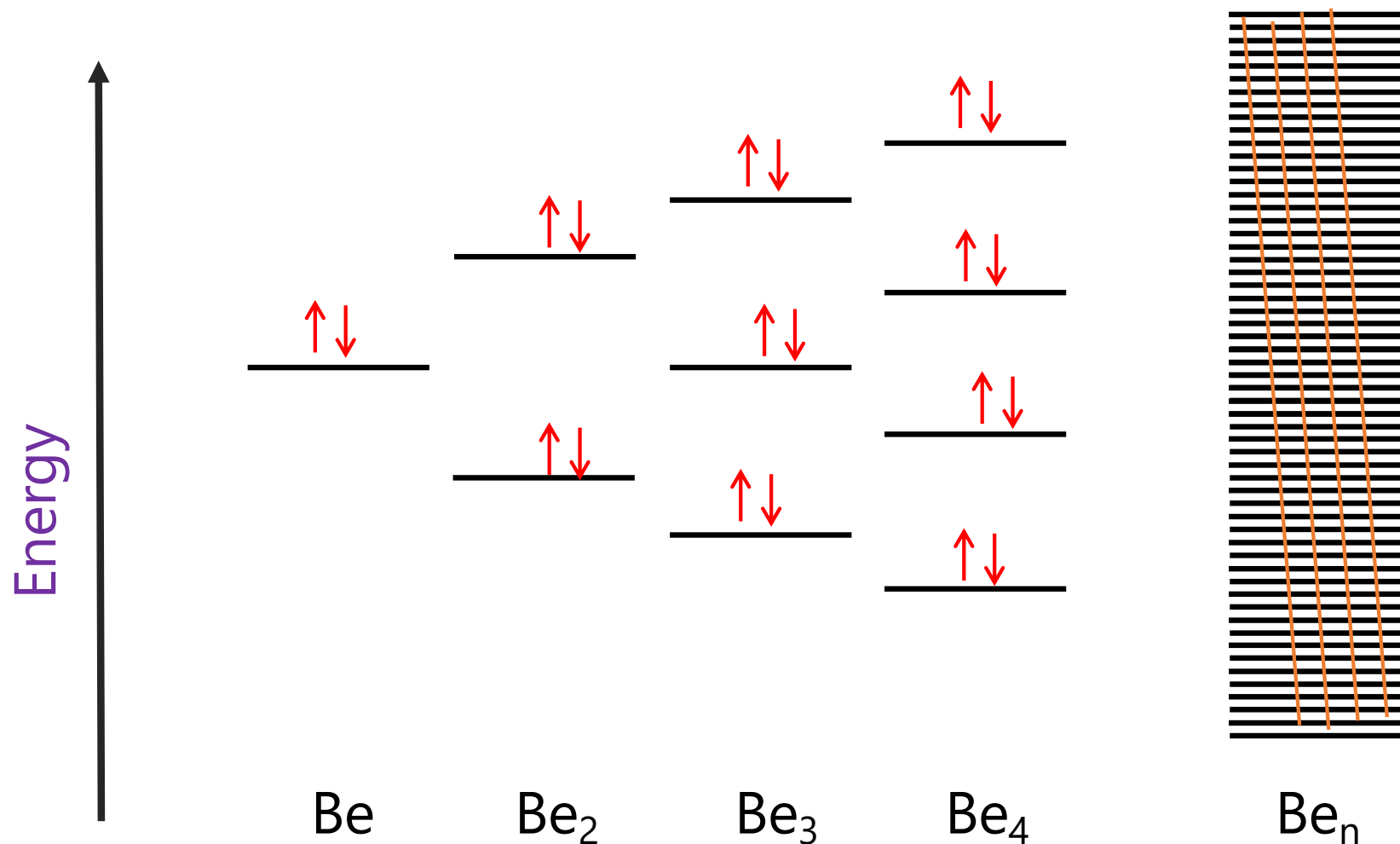
* Small energy gaps enable easy excitation and "mobile" electrons *
(partially filled energy band enables conductivity)

Be₂ MO Energy Diagram



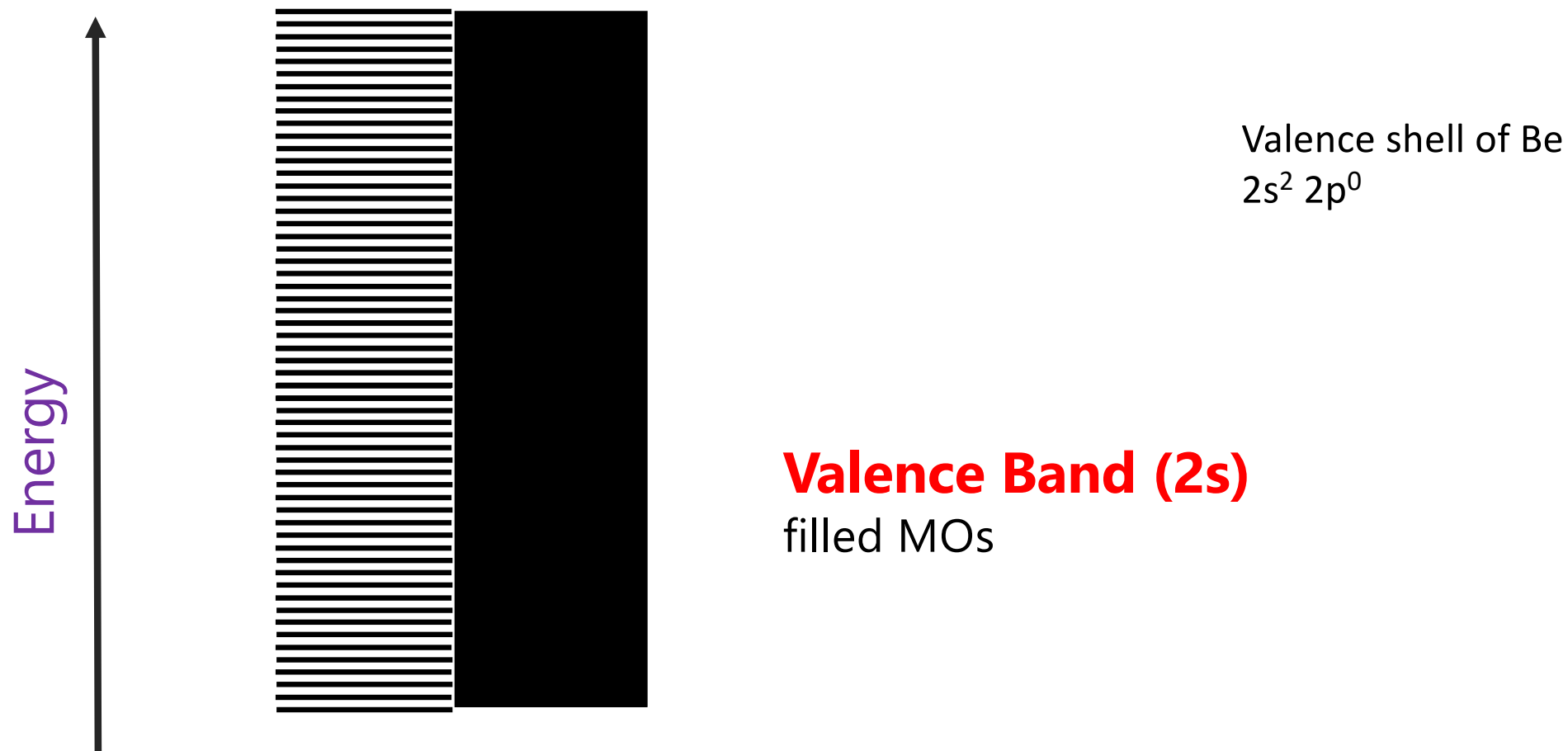
Band Theory Group 2 Metals

Be_n (metal): *n* 2s AOs = *n* MOs (2*n* valence electrons)



Be: Only using 2s Energy Band

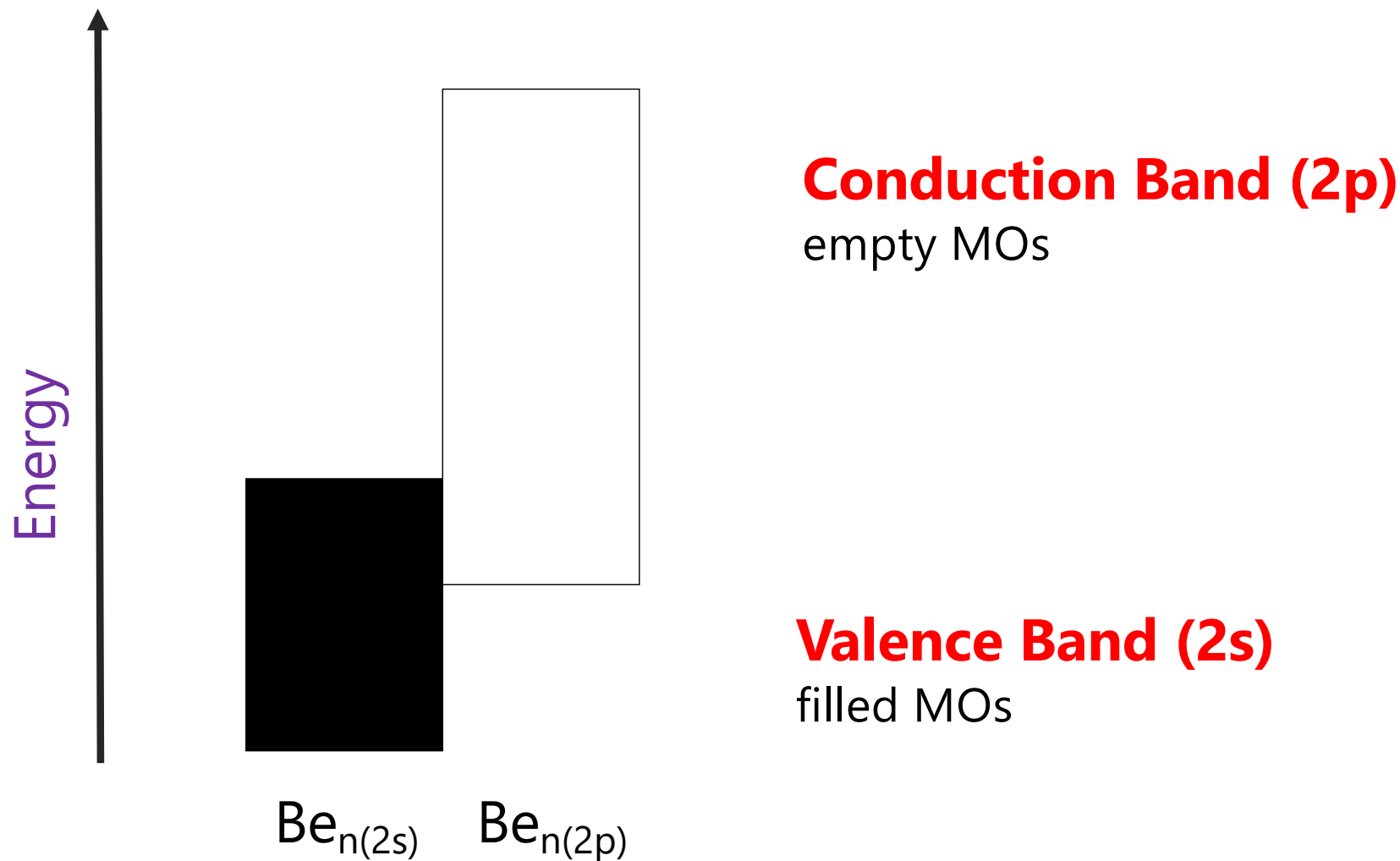
Be_n (metal): *n* 2s AOs = *n* MOs (2*n* valence electrons)



* 2s band completely filled... but 2p band is empty!*

Be with 2s and 2p Energy Bands

Be_n (metal): n 2s + $3n$ 2p AOs = $4n$ MOs ($2n$ valence electrons)



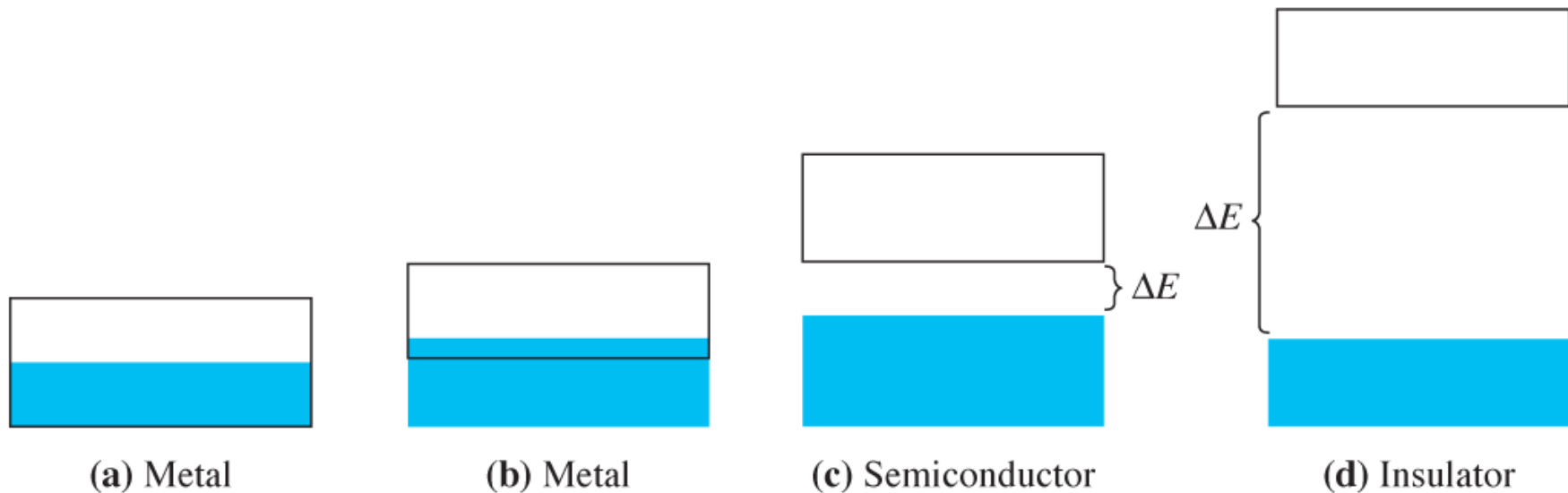
Conductivity

Conductivity depends upon the size of the energy “gap” between valence and conduction band

Metals(conductors) – no band gap, “free” electrons (no covalent bonds)

Semiconductors – small band gap, bonding has more covalent character

Insulators – large band gap, strongly held electrons in covalent bonds



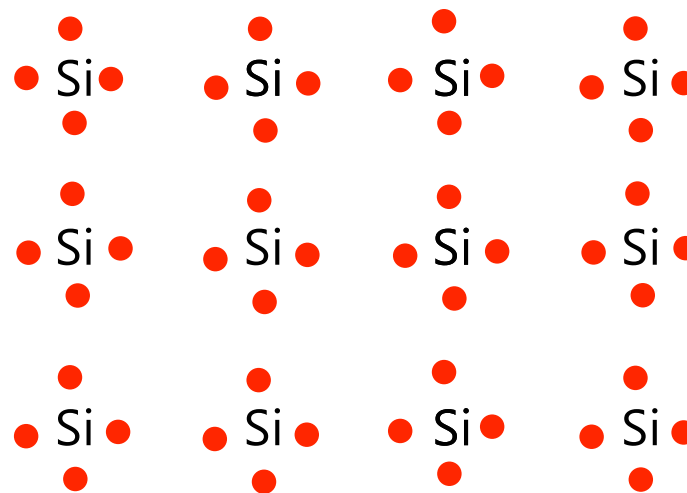
Semiconductors

Si_n (semimetal) – intrinsic semiconductor (fixed band gap)

4n AOs = 4n MOs (4n valence electrons)



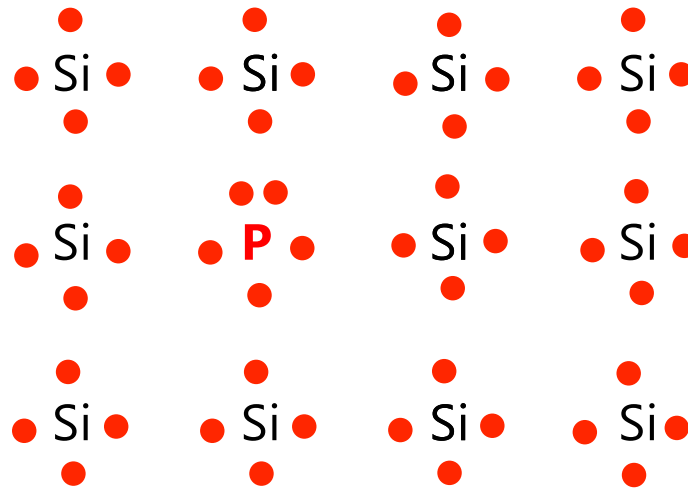
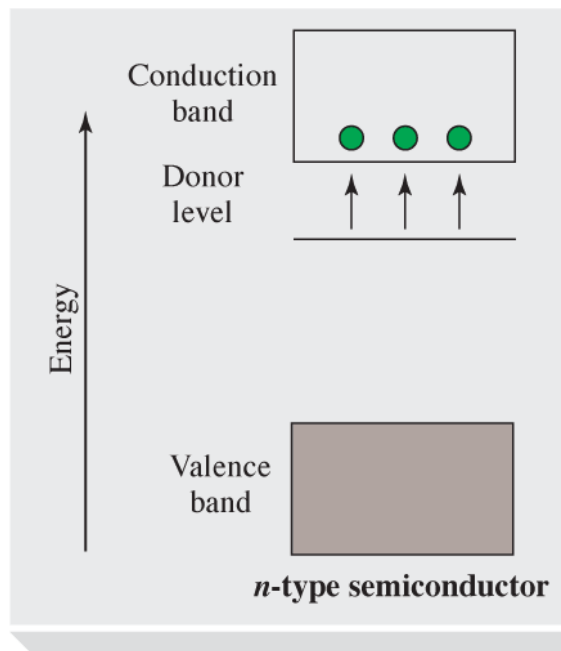
(c) Semiconductor



*** more electrons can be excited to conduction band when more energy applied ***

“Doped” Semiconductors: Si/P

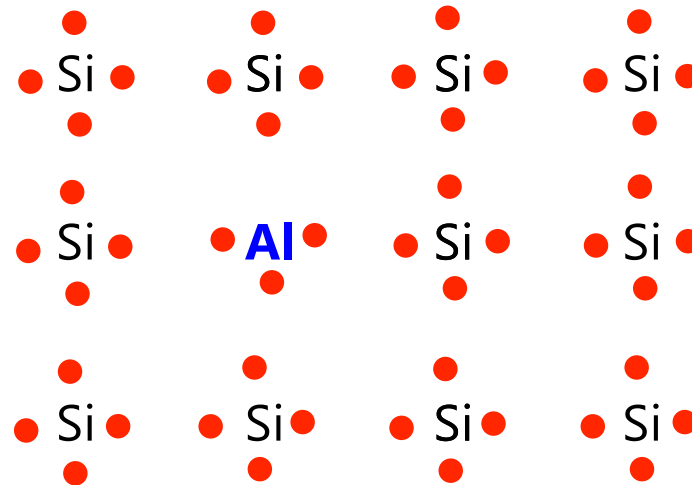
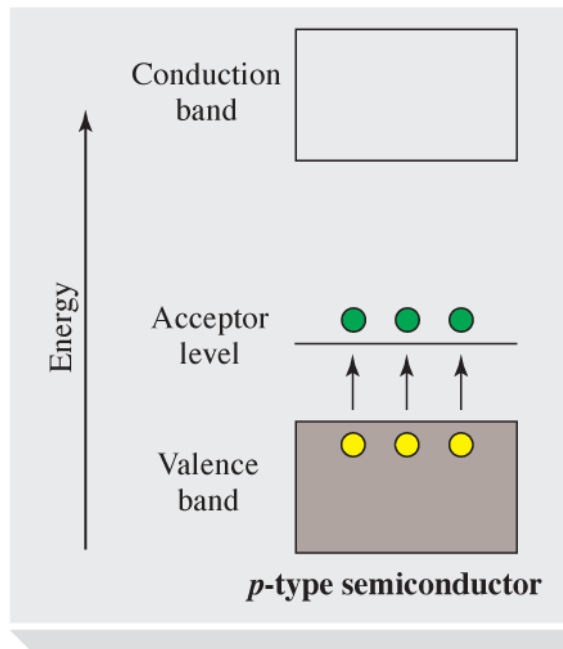
Si_n doped with P – extrinsic semiconductor (altered band gap)
(n-type semi-conductor – “negative” from extra P electron)

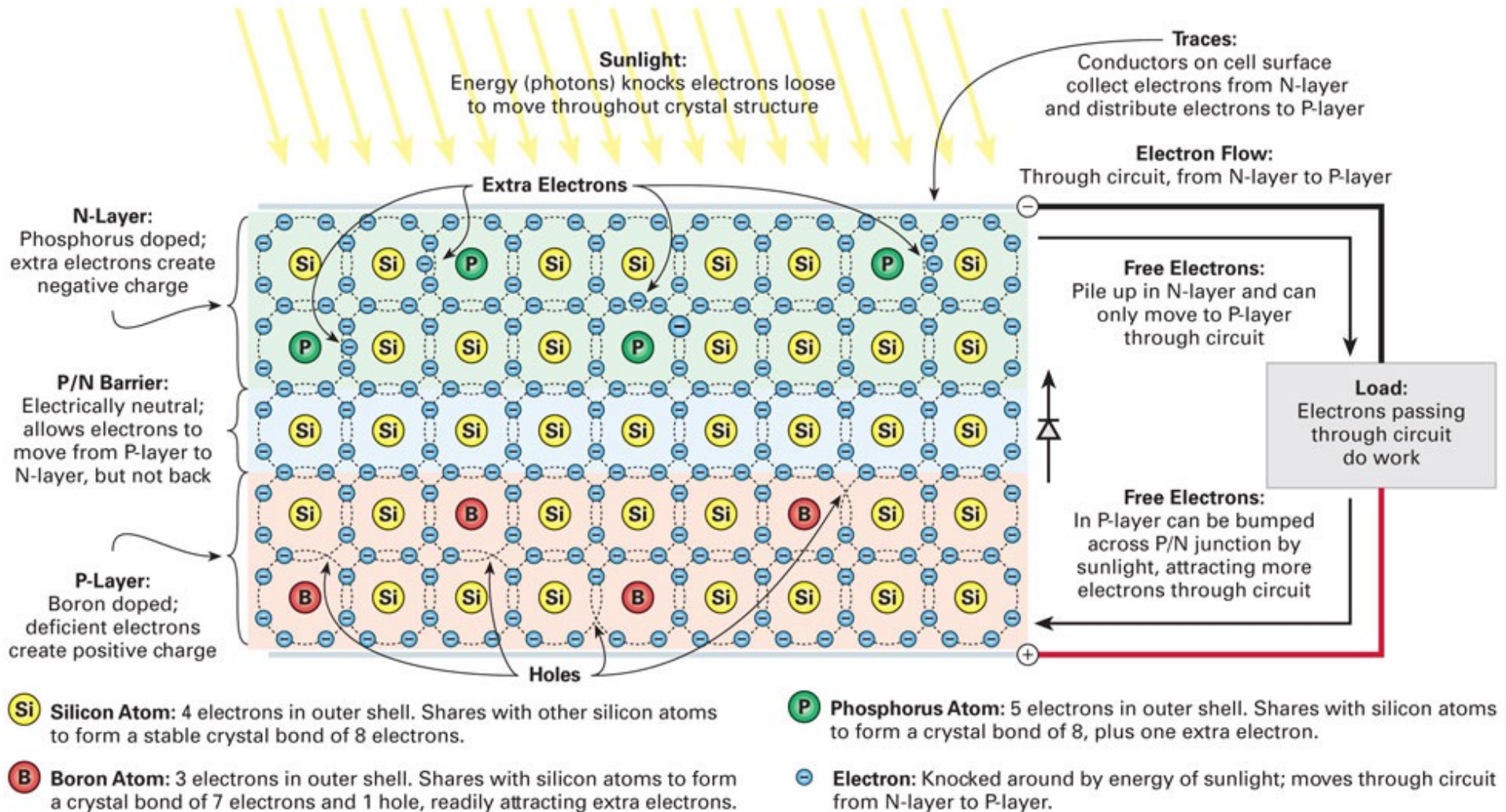


*** more electrons can be excited to conduction band when more energy applied ***

“Doped” Semiconductors – Si/Al

Si_n doped with Al – extrinsic semiconductor (altered band gap)
(p-type semi-conductor – “positive” from missing Al electron)





<http://www.homepower.com/articles/solar-electricity/equipment-products/peek-inside-pv-cell>