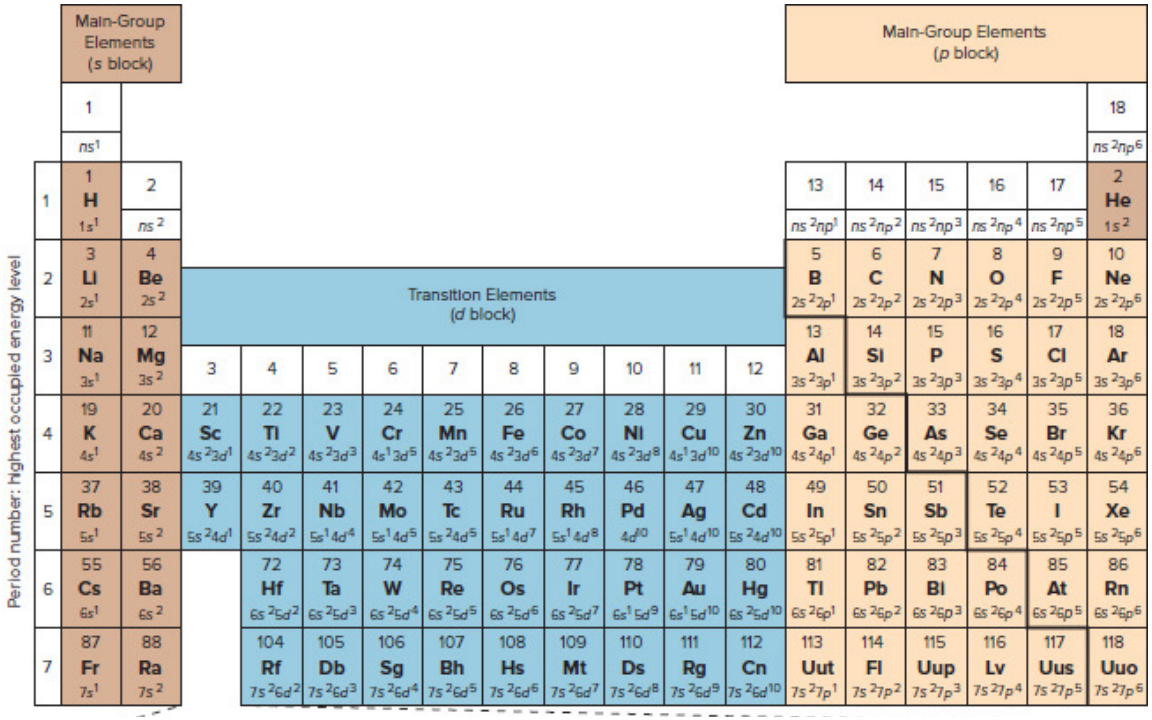
Applying MO theory to other systems

Conducting materials (metals/semiconductors) show similar behaviour

Metallic Properties

Metallic Character decreases

Metallic character increases

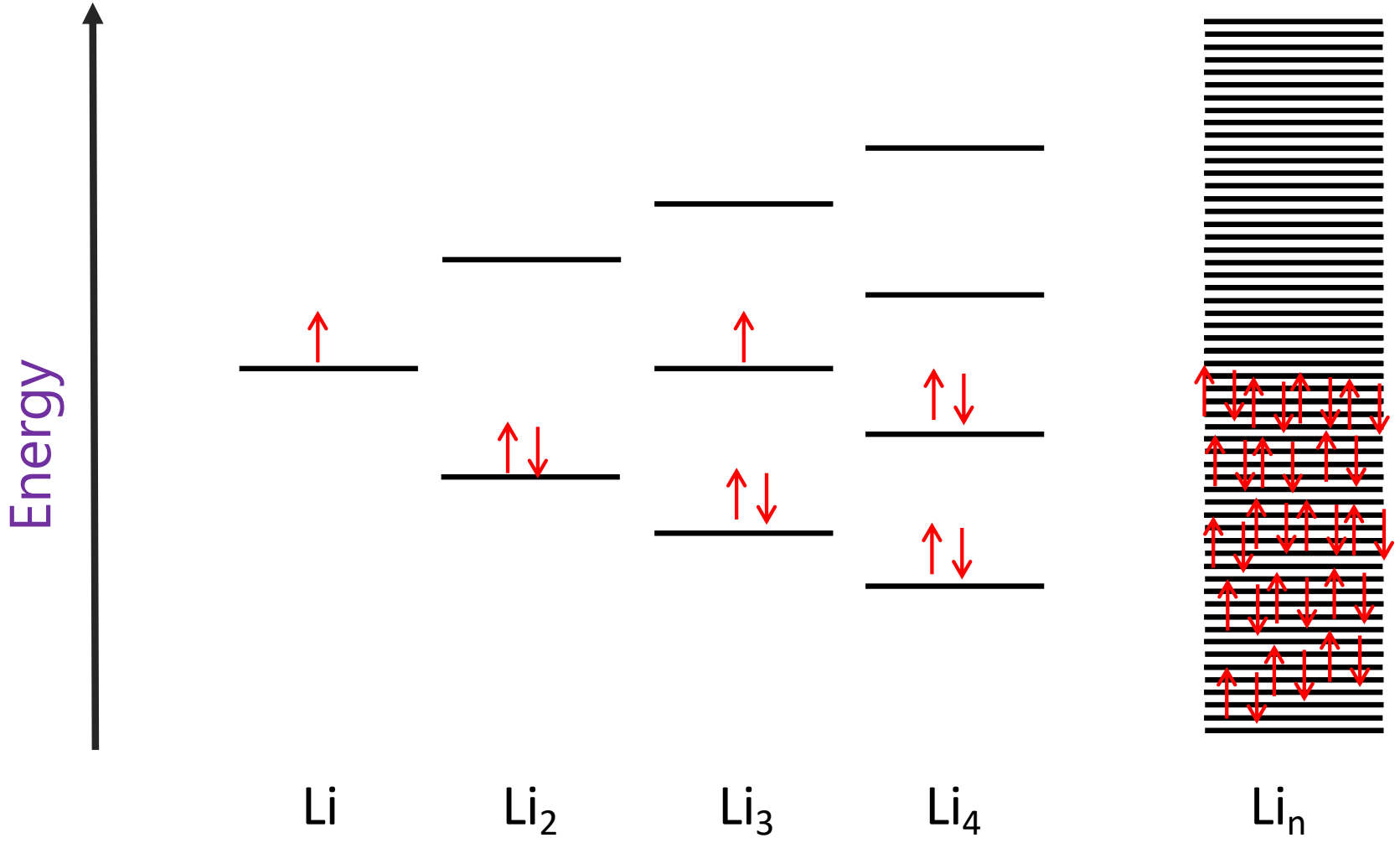


Metals

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

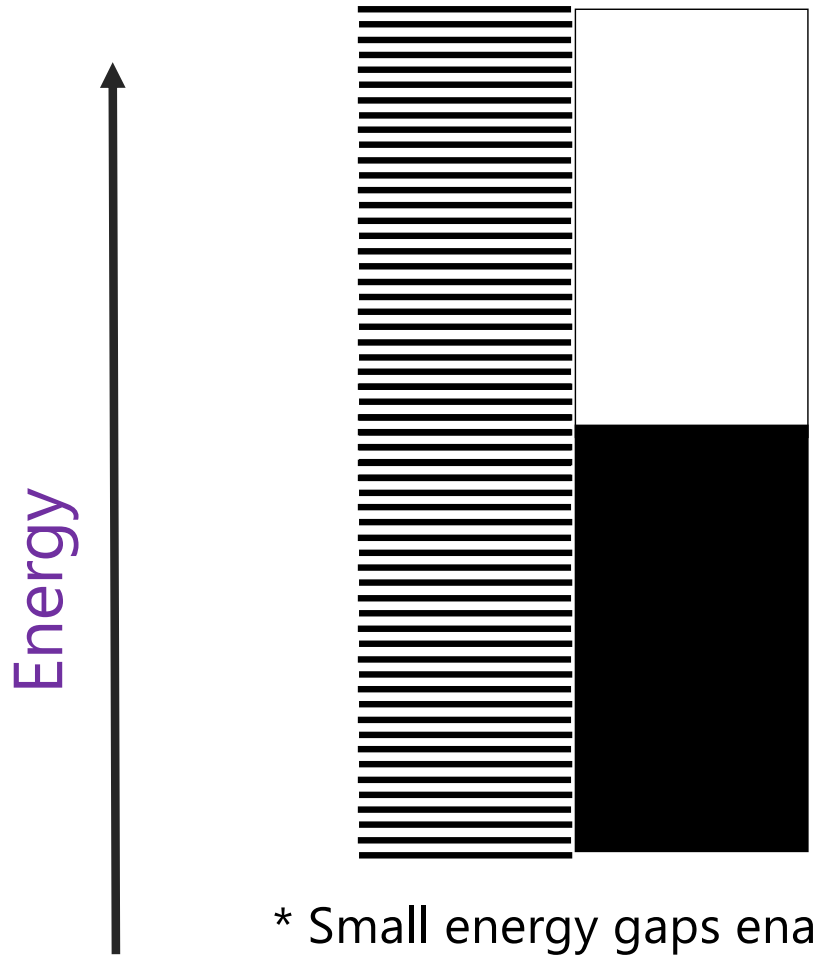
Band Theory: Group 1 Metals

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)

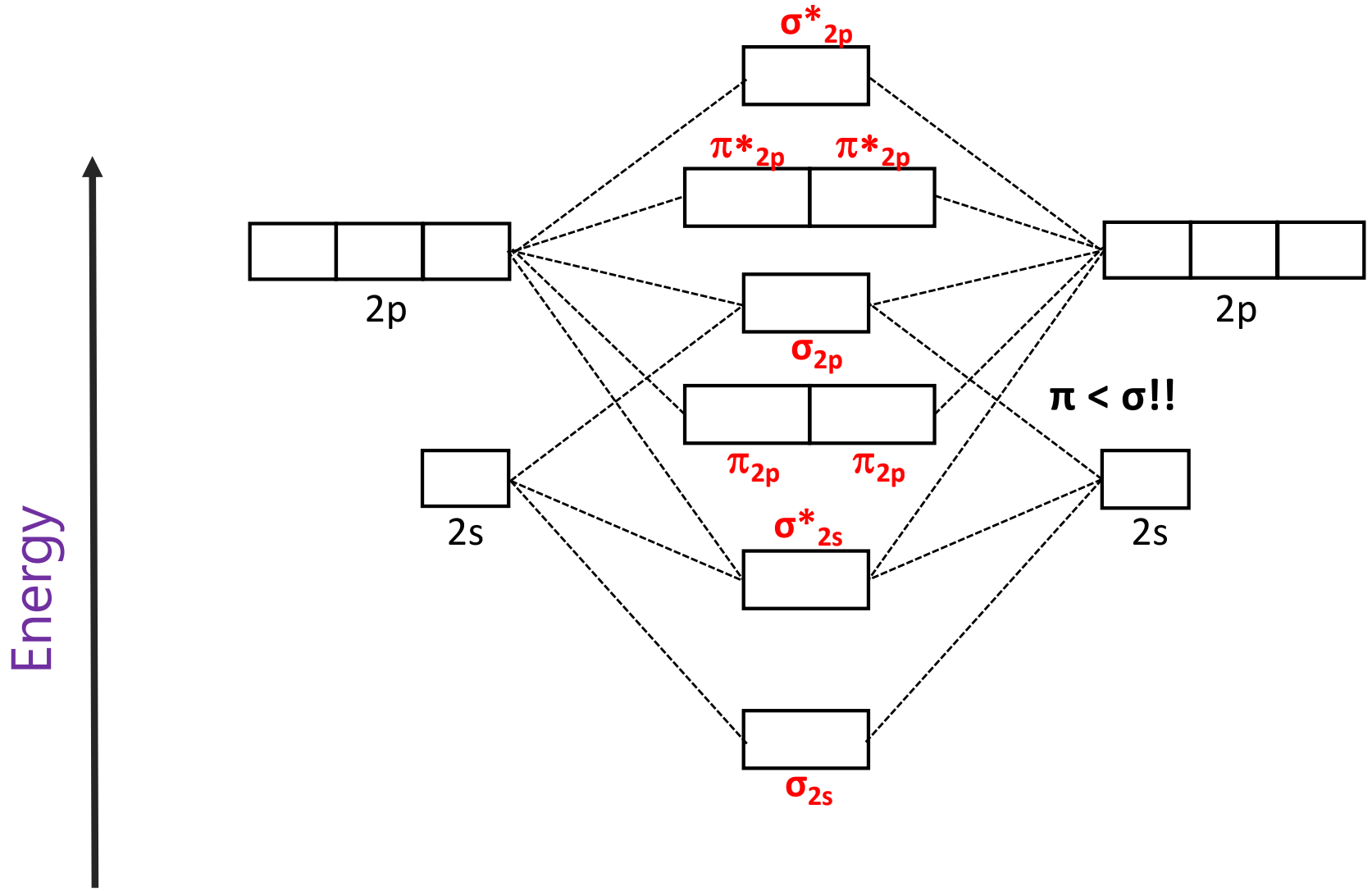


Conduction Band
empty MOs

Valence Band
filled MOs

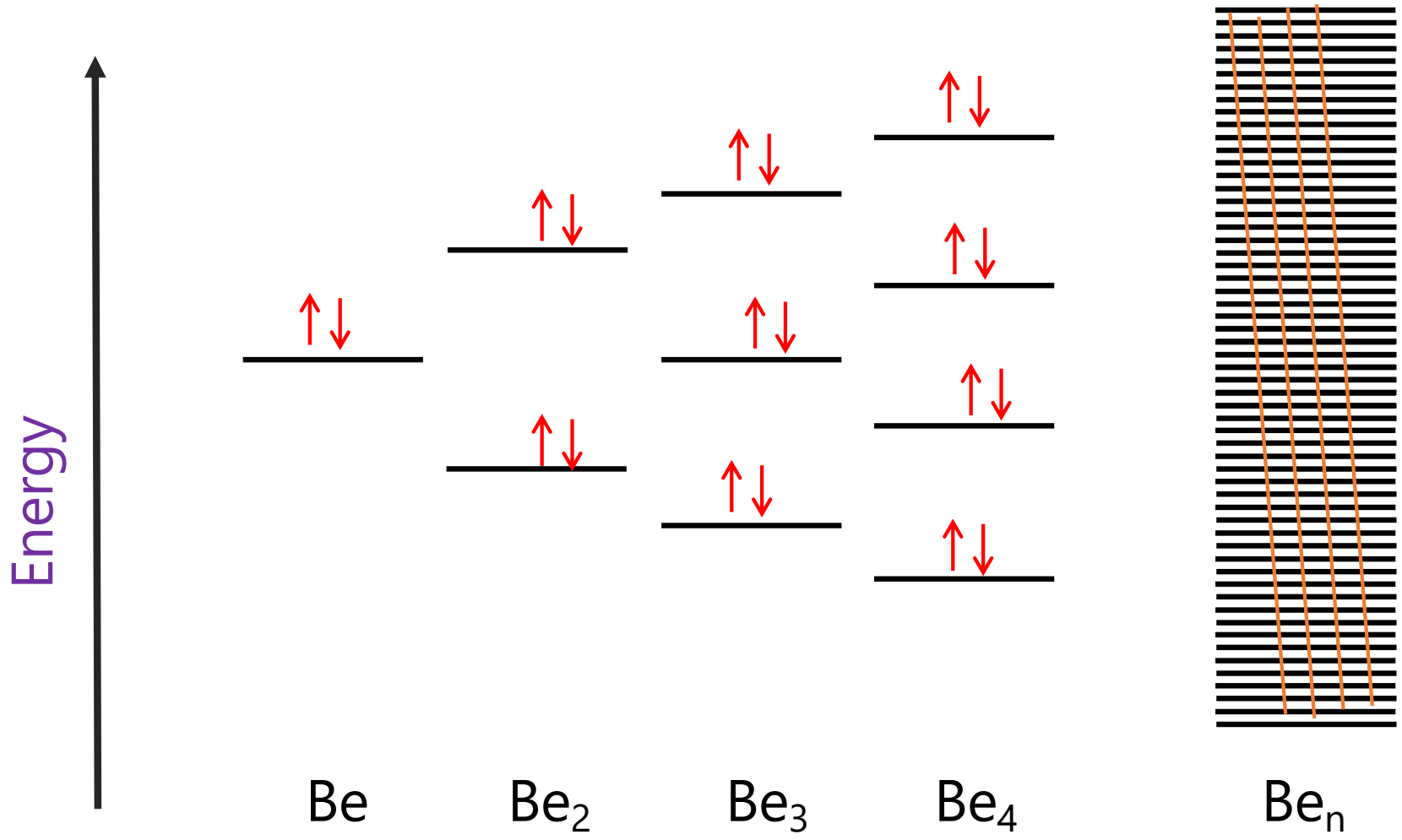
* Small energy gaps enable easy excitation and "mobile" electrons *
(partially filled energy band enables conductivity)

Be_2 MO Energy Diagram



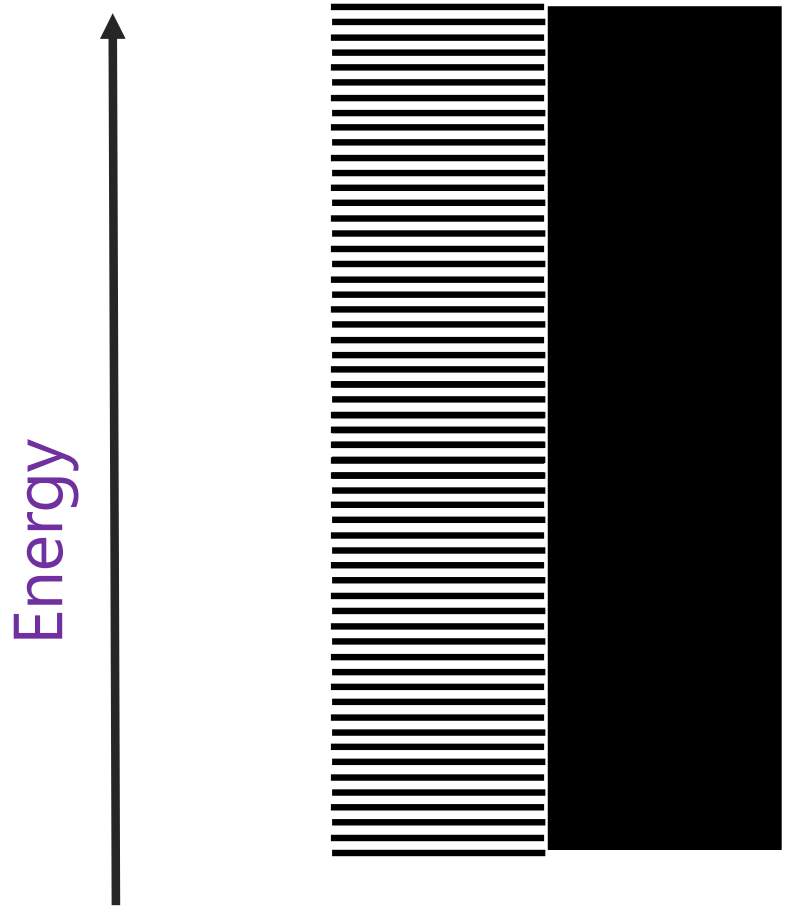
Band Theory Group 2 Metals

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



Be: Only using 2s Energy Band

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



Valence shell of Be
$2s^2\ 2p^0$

Valence Band (2s)
filled MOs

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

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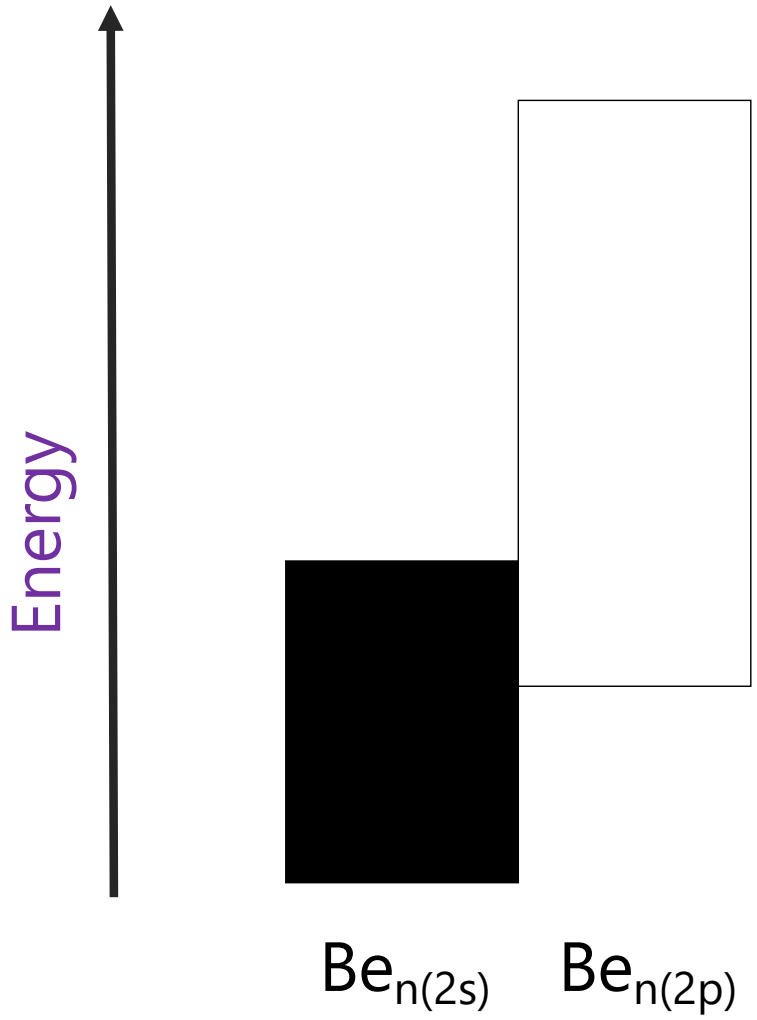
Be with 2s and 2p Energy Bands

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



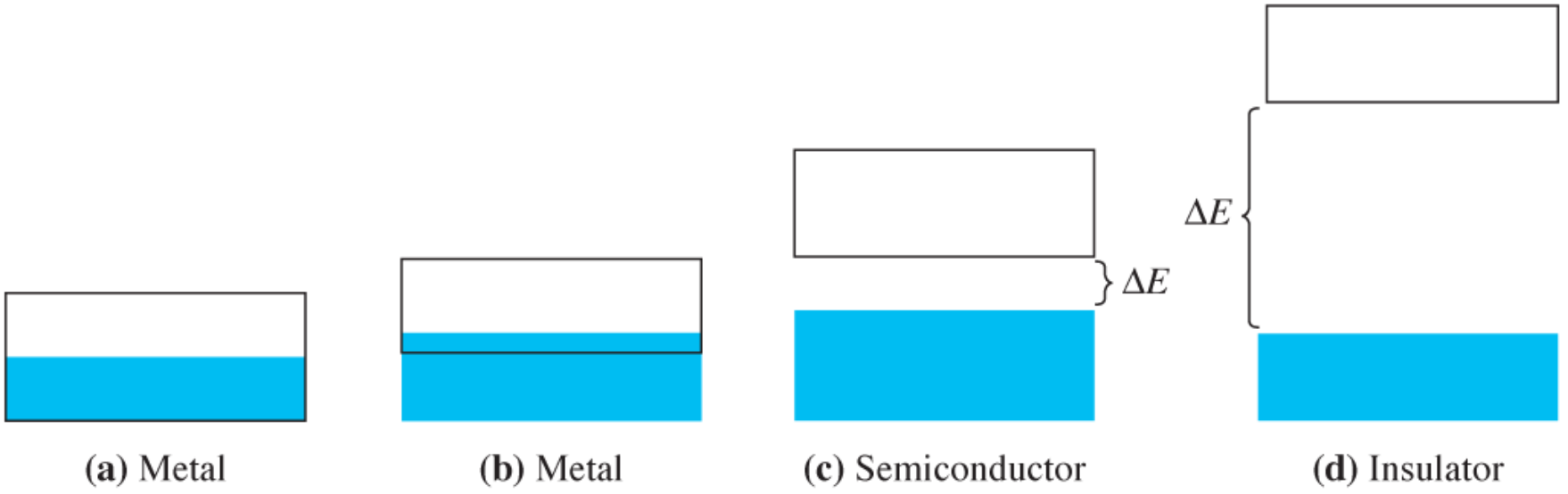
Conduction Band (2p)
empty MOs

Valence Band (2s)
filled MOs

Conductivity

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

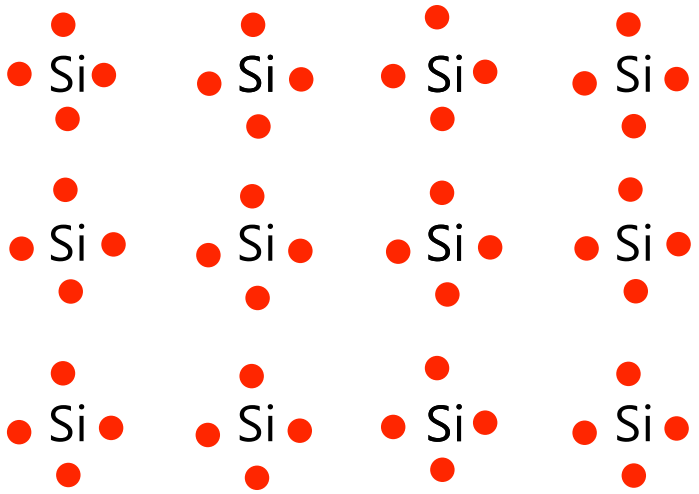
Metals(conductors) – no band gap, "free" electrons (no covalent bonds)
Semiconductors – small band gap, bonding has more covalent character
Insulators – large band gap, strongly held electrons in covalent bonds



Semiconductors

Si_n (semimetal) – intrinsic semiconductor (fixed band gap)
4n AOs = ***4n*** MOs (***4n*** valence electrons)

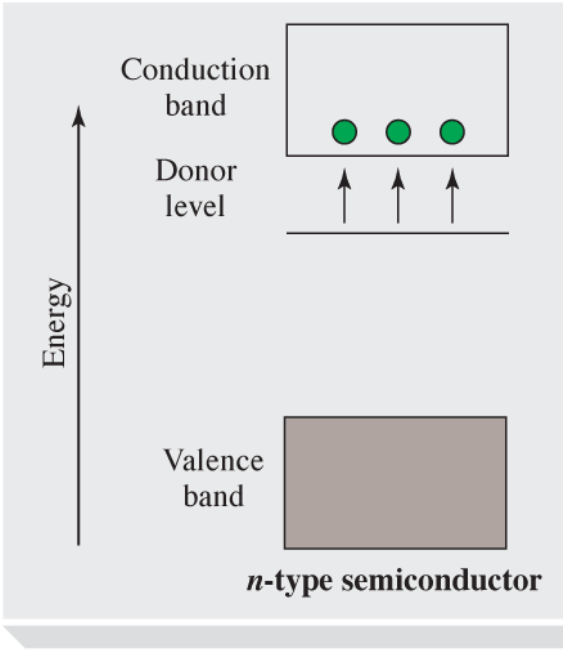
(c) Semiconductor

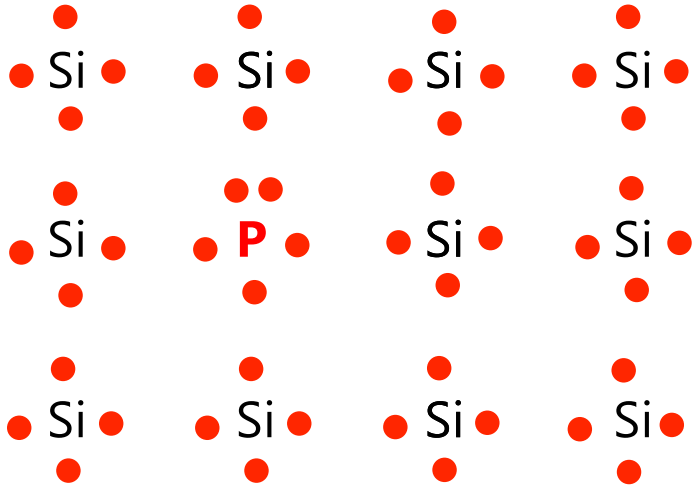


*** more electrons can be excited to conduction band when more energy applied ***

“Doped” Semiconductors: Si/P

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

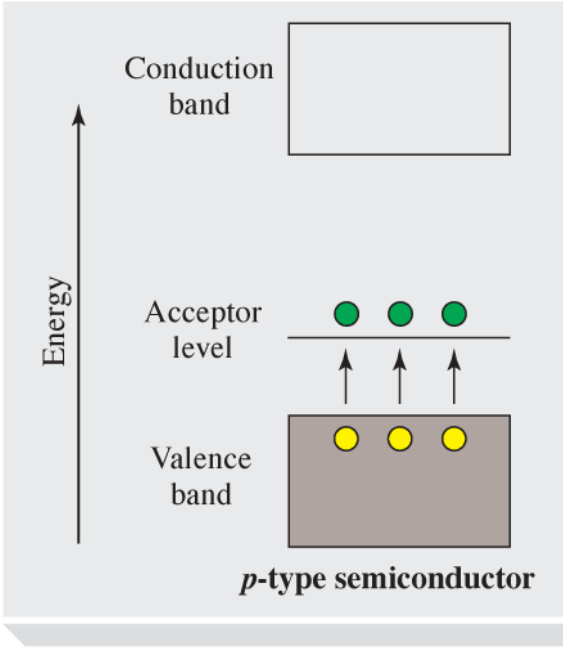


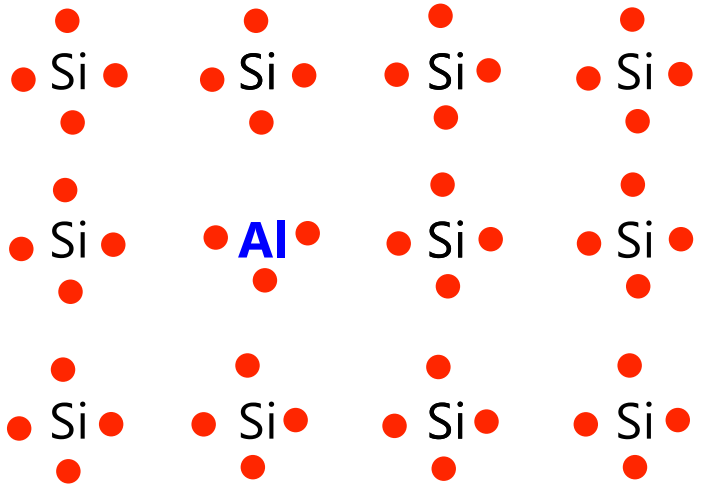


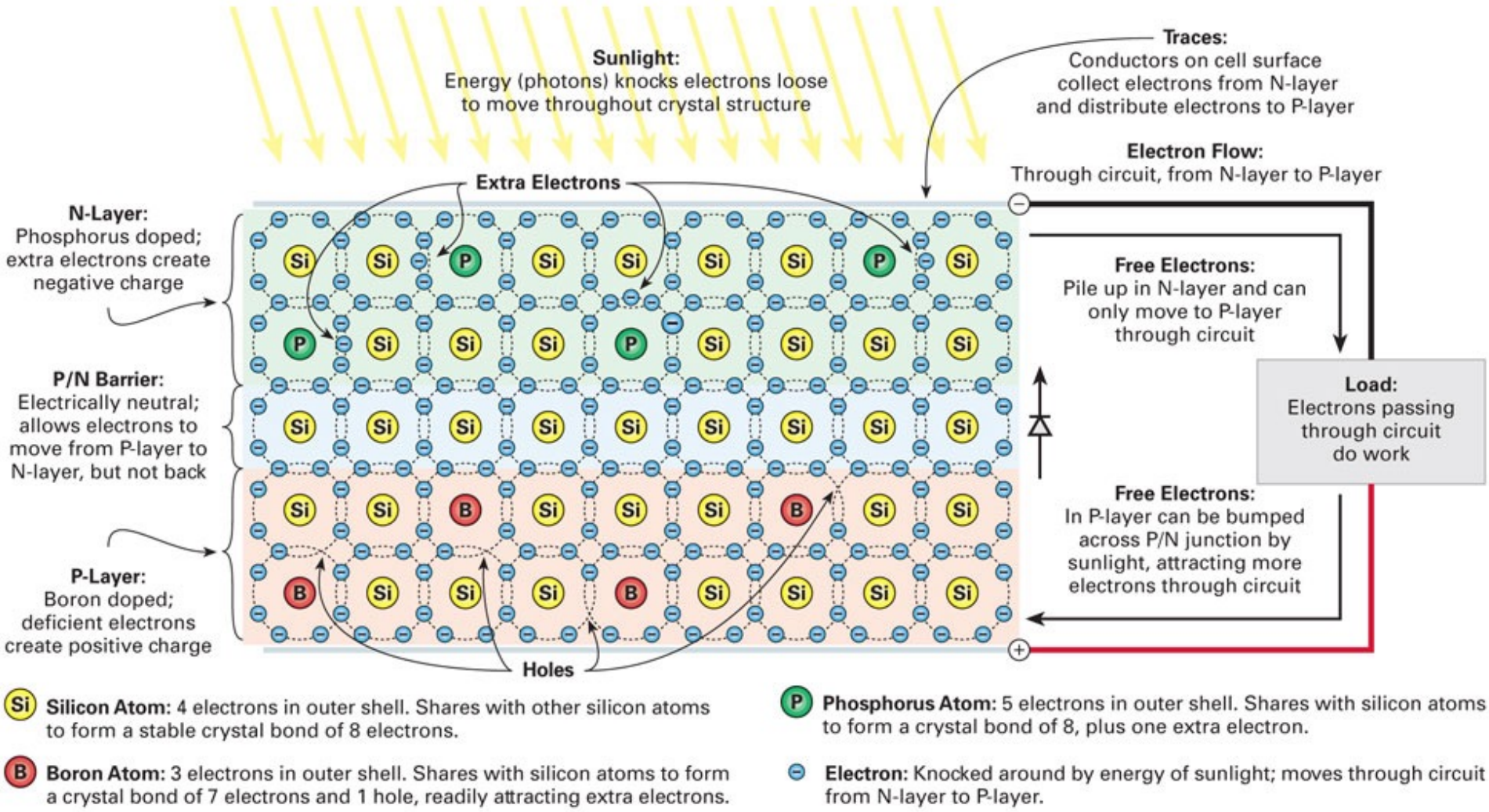
*** more electrons can be excited to conduction band when more energy applied ***

“Doped” Semiconductors – Si/Al

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







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