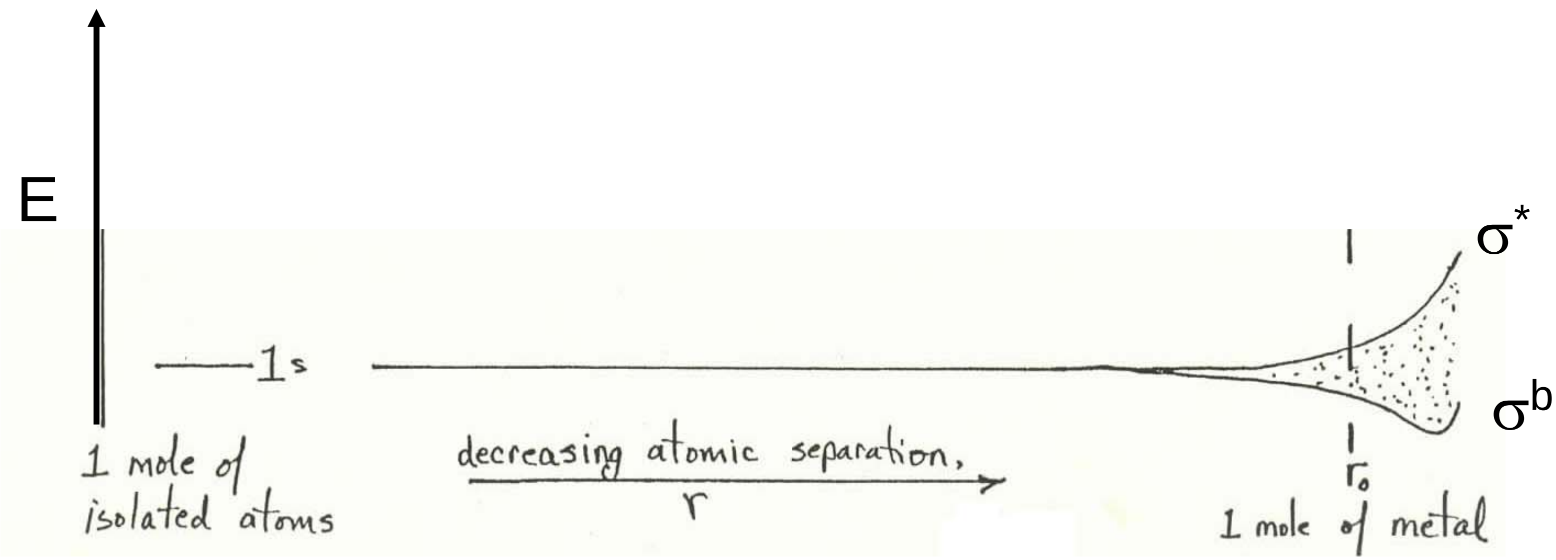
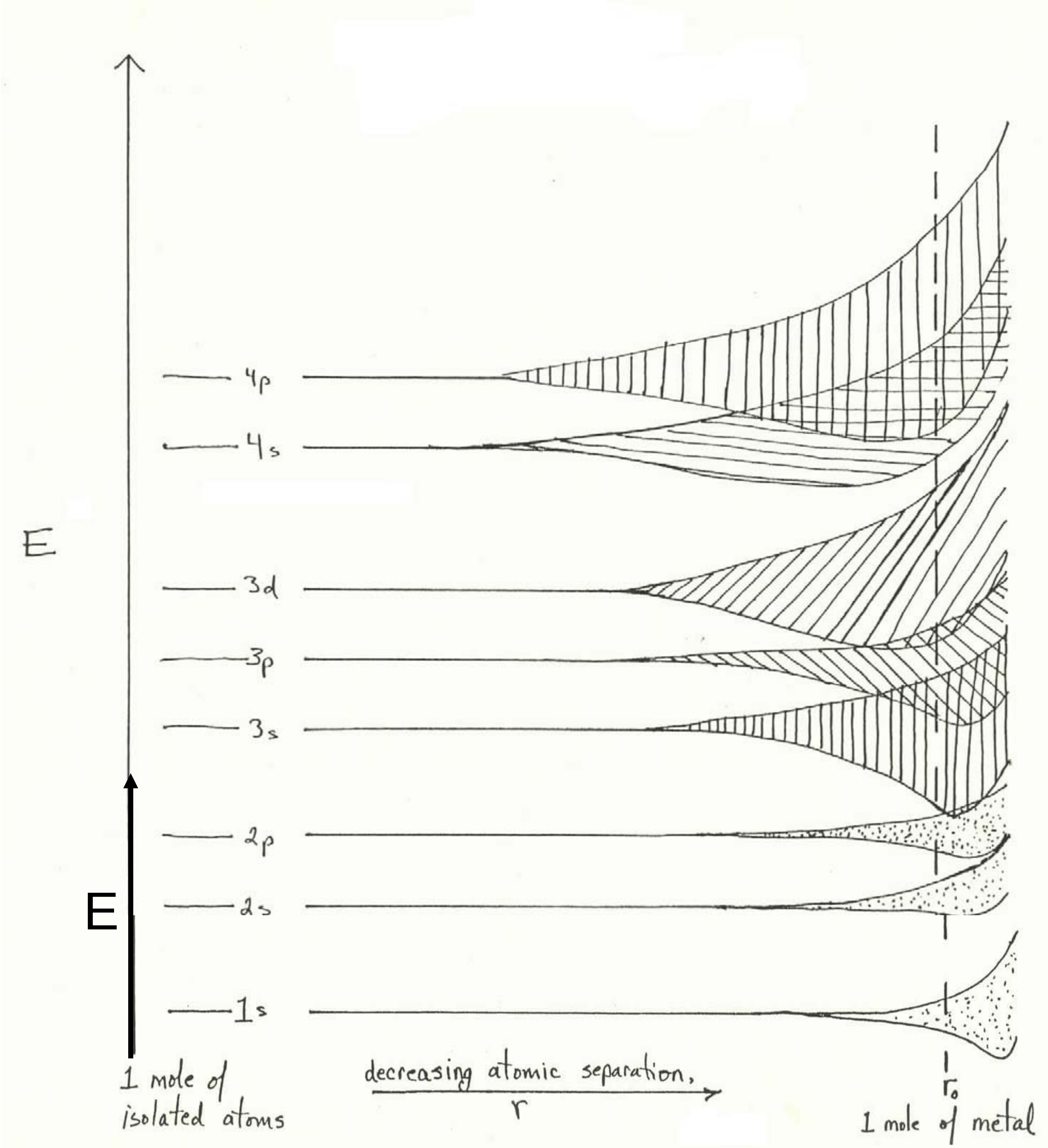
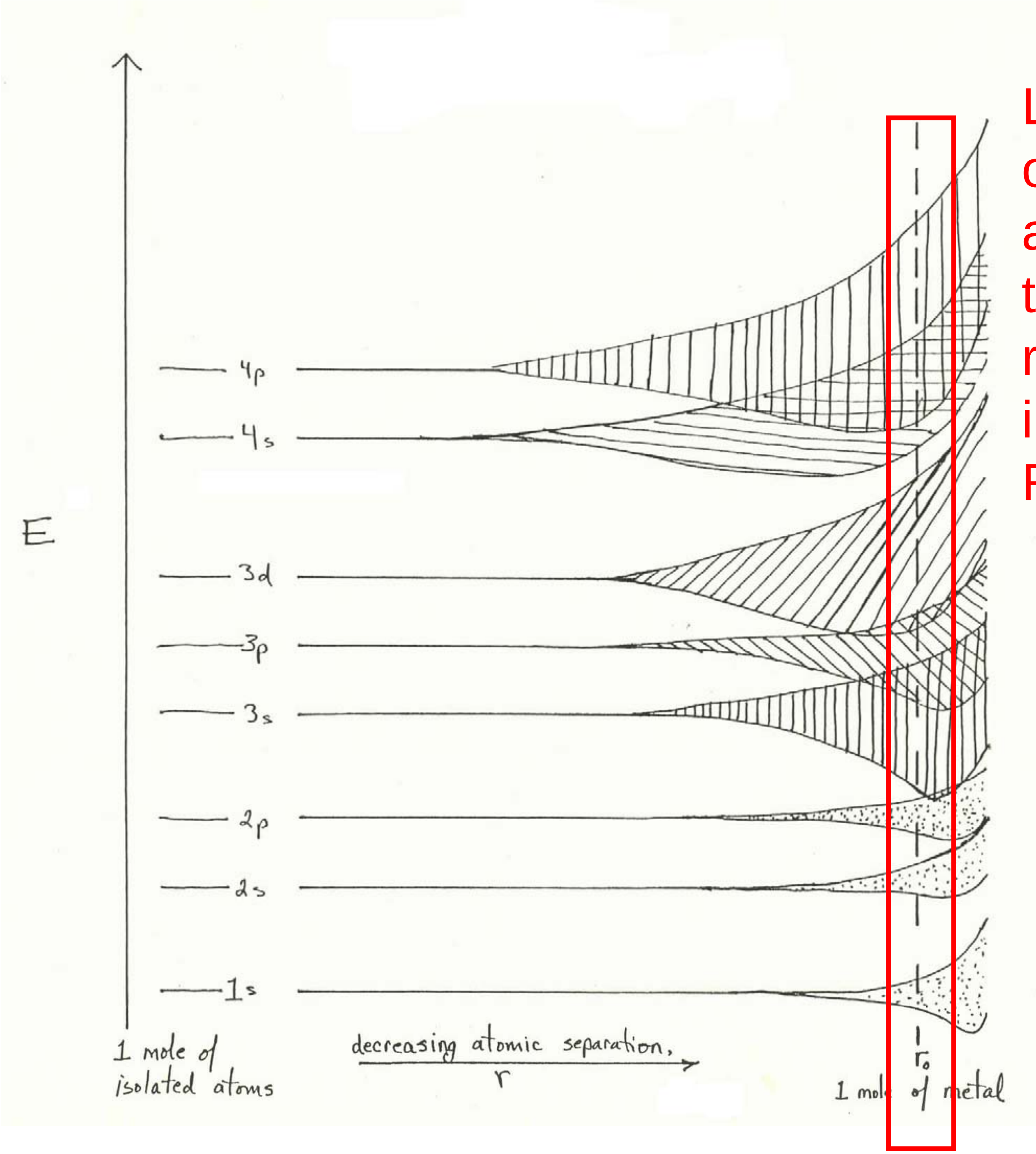

E
1s
σ*
σb
1 mole of isolated atoms
decreasing atomic separation, r
r₀
1 mole of metal

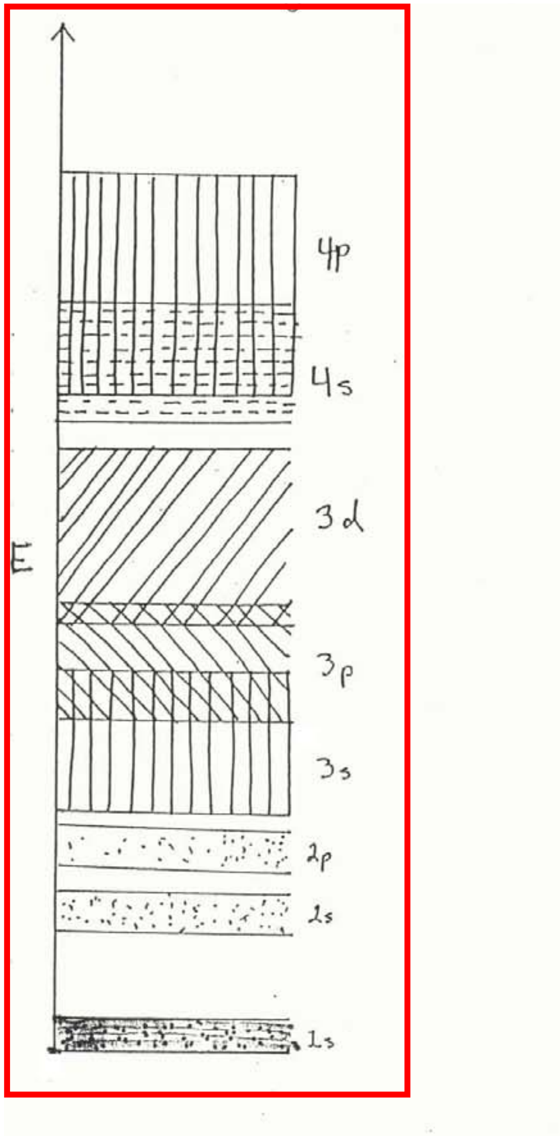


E
4p
4s
3d
3p
3s
2p
2s
1s
E
1 mole of isolated atoms
decreasing atomic separation, r
r_0
1 mole of metal

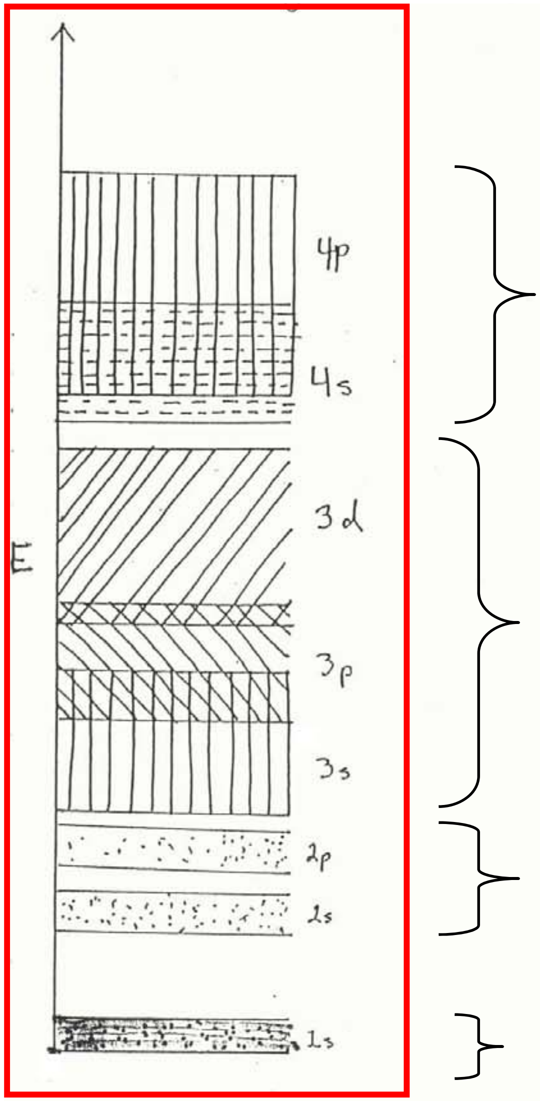


Looking only at this region in the Rectangle:

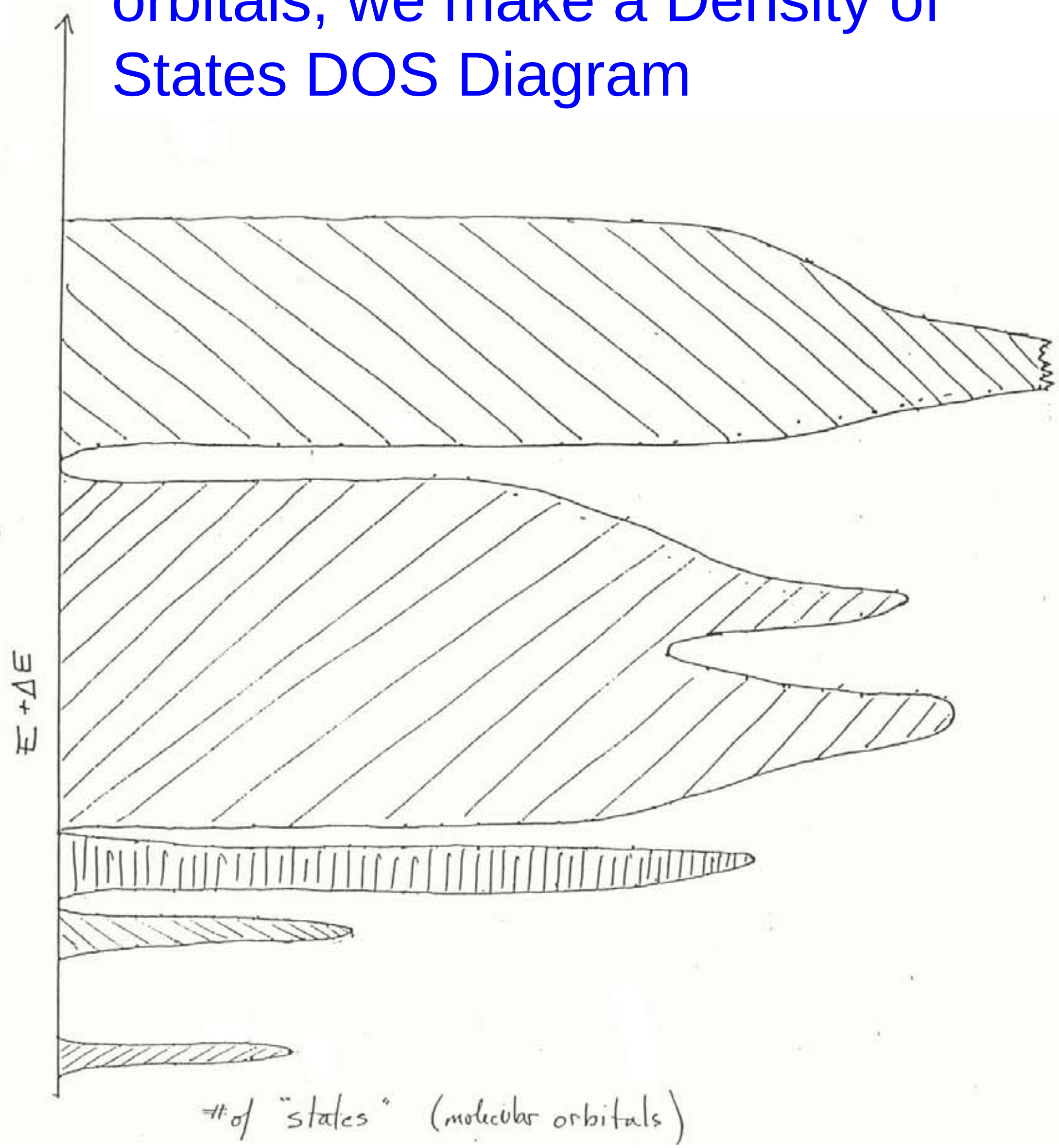
We generated a Band Diagram



We generated a Band Diagram



If we include the relative number of orbitals, we make a Density of States DOS Diagram



We do the same thing again, starting with isolated atoms,
Then turn on the bonding, then increase the number of interacti

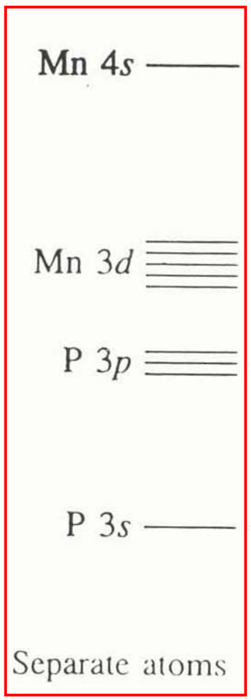
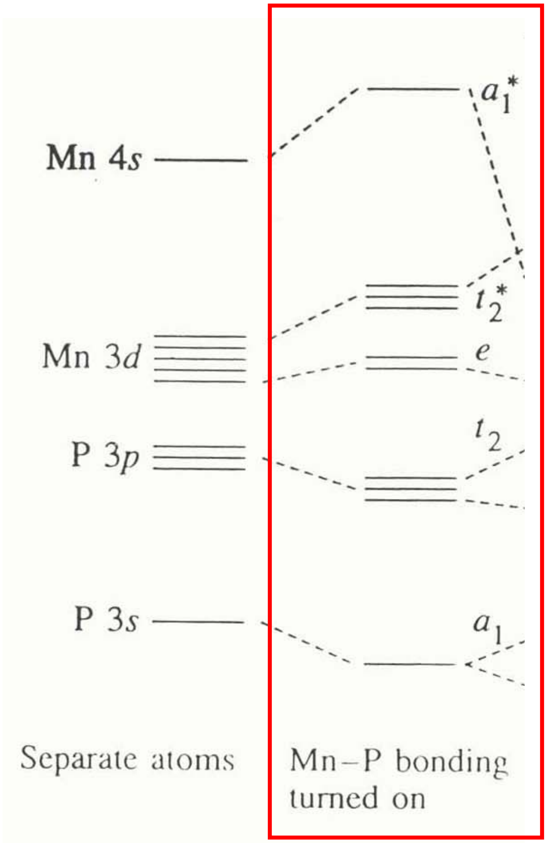
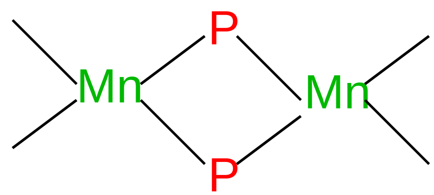


Fig. 7.29 Left: Energy levels of separated Mn and P atoms, Mn–P MO's from adjacent atoms, and extended bonding. Right: Band structure of a single $[Mn_2P_2]_\infty^{2-}$ layer. [Modified from Hoffmann, R.; Zheng, C. *J. Phys. Chem.* **1985**, *89*, 4175–4181. Reproduced with permission.]





Polymeric unit

Fig. 7.29 Left: Energy levels of separated Mn and P atoms, Mn–P MO's from adjacent atoms, and extended bonding. Right: Band structure of a single $[Mn_2P_2]_\infty^{2-}$ layer. [Modified from Hoffmann, R.; Zheng, C. *J. Phys. Chem.* **1985**, *89*, 4175–4181. Reproduced with permission.]

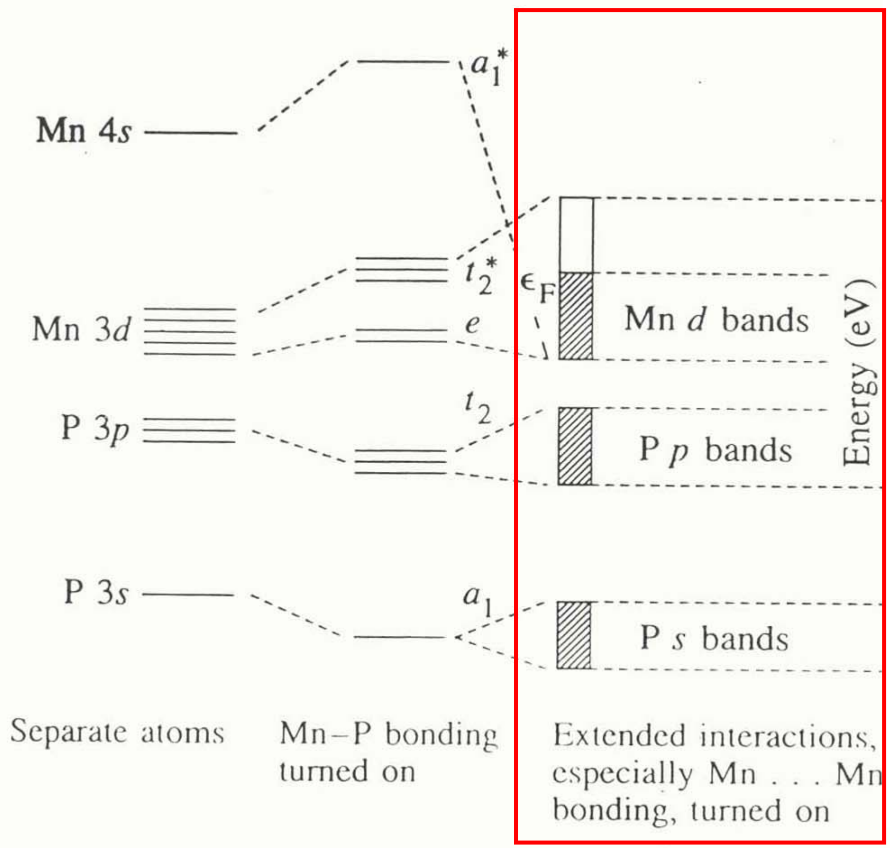


Fig. 7.29 Left: Energy levels of separated Mn and P atoms, Mn–P MO's from adjacent atoms, and extended bonding. Right: Band structure of a single $[Mn_2P_2]_x^{2-}$ layer. [Modified from Hoffmann, R.; Zheng, C. *J. Phys. Chem.* **1985**, *89*, 4175–4181. Reproduced with permission.]

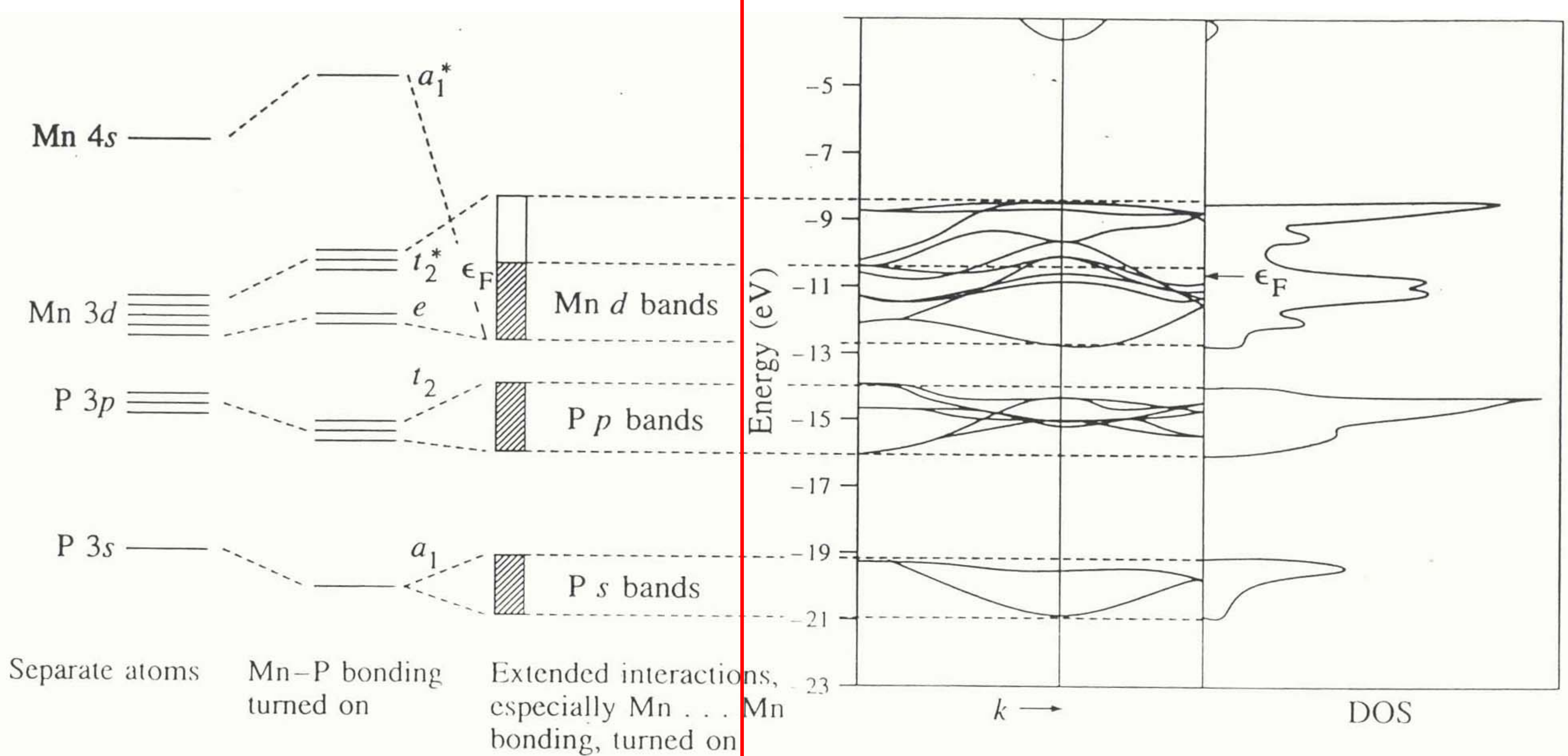


Fig. 7.29 Left: Energy levels of separated Mn and P atoms, Mn–P MO's from adjacent atoms, and extended bonding. Right: Band structure of a single $[Mn_2P_2]_\infty^{2-}$ layer. [Modified from Hoffmann, R.; Zheng, C. *J. Phys. Chem.* **1985**, *89*, 4175–4181. Reproduced with permission.]

An actual example, calculated using an M.O.theory

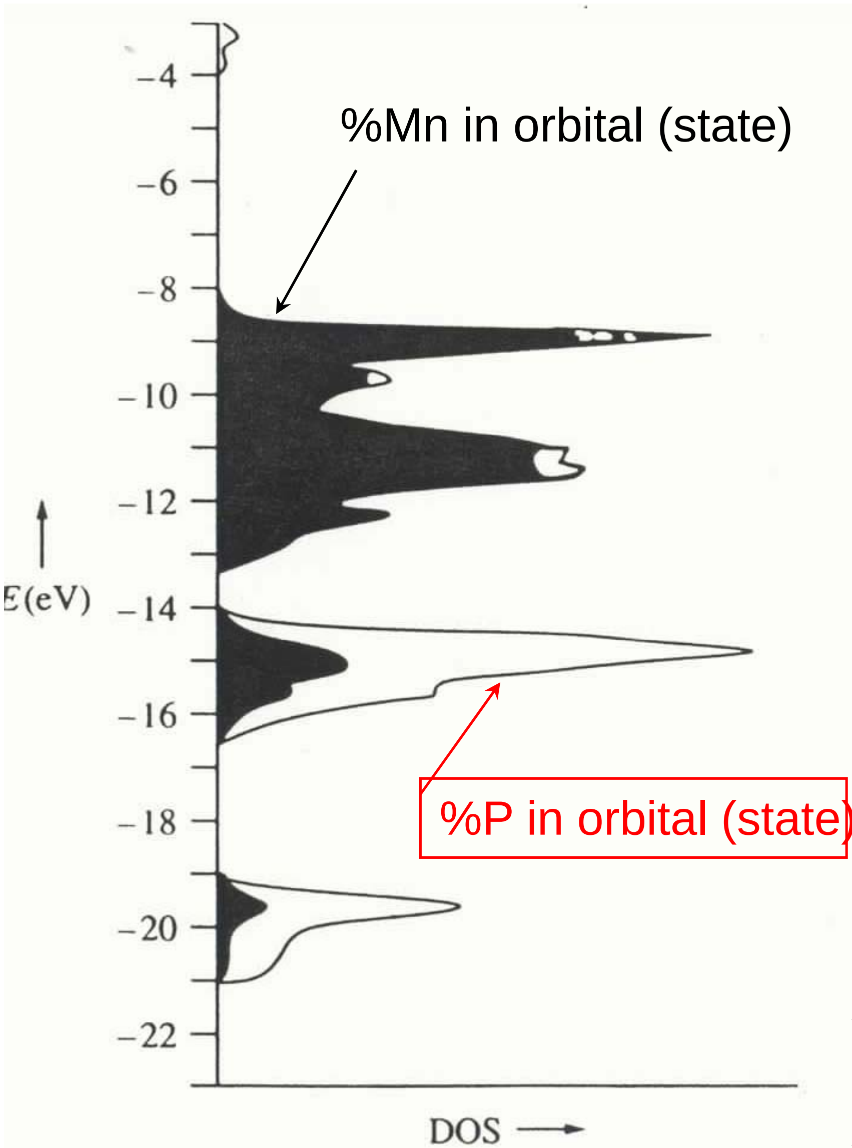
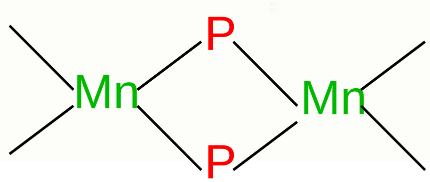


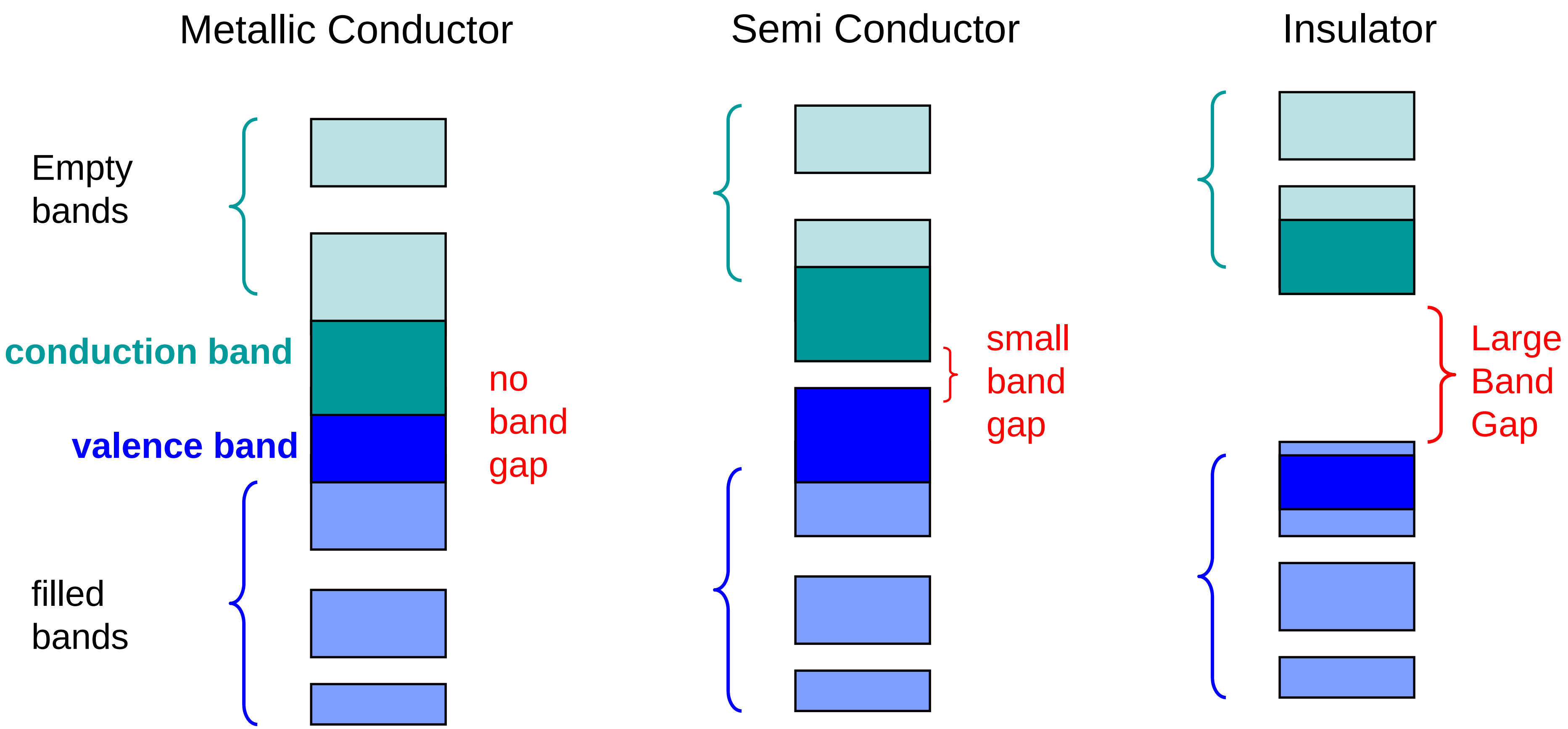
Fig. 7.30 Total DOS of the extended $[Mn_2P_2]_x^{2-}$ layer. The relative contributions of the manganese (dark area) and the phosphorus (light area) are indicated. Note that the bonding states at −19 and −15 eV are dominated by the phosphorus, that is, there is more electron density on the phosphorus than on the manganese. [From Hoffmann, R.; Zheng, C. *J. Phys. Chem.* **1985**, *89*, 4175–4181. Reproduced with permission.]



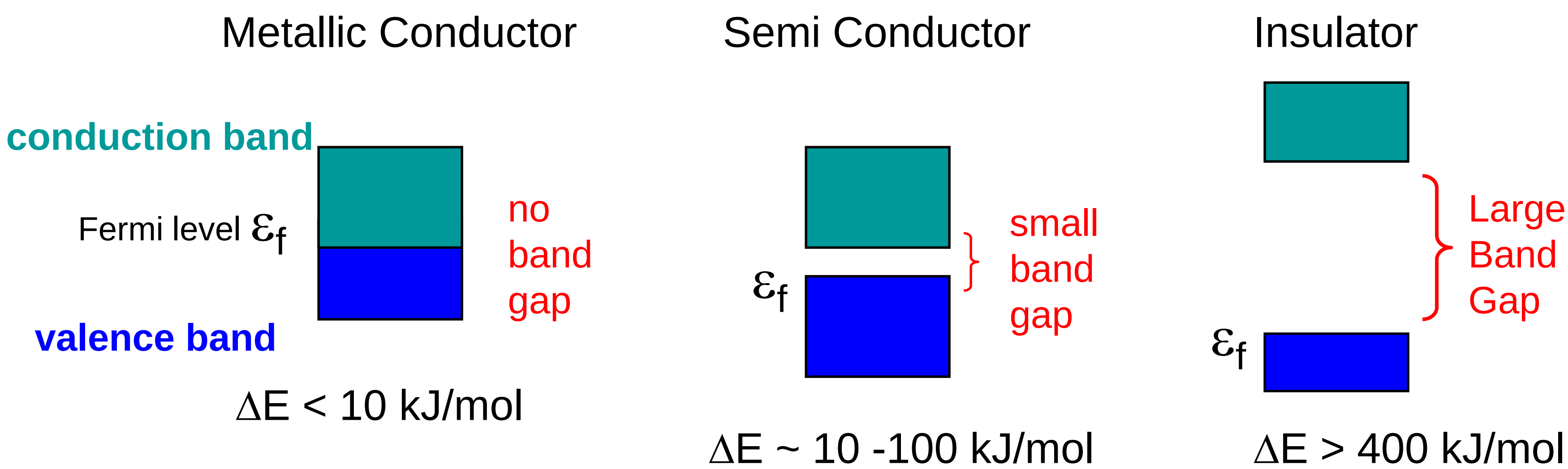
Polymeric unit

MOT analogies with Band Diagram

- HOMO / LUMO and type of reactivity
- Valence Band / Conduction band and
- DE and Band Gap

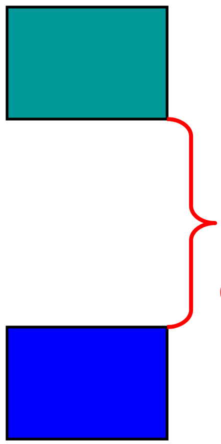


More typically simplified to show only "frontier" bands:



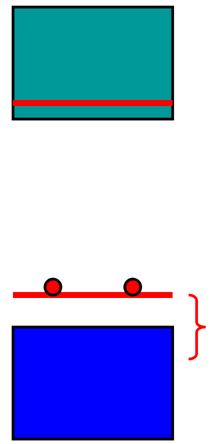
How Defects Improve Semi-Conduction

Pure Germanium



$\Delta E \sim 0.66$ eV

Gallium-Doped Ge



Ga more
Electropositive:

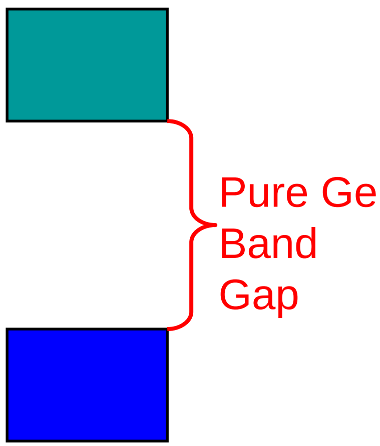
Adds “Orbitals”
At Higher
Energy
With Fewer
Electrons

Gallium-Doping creates positive holes,
as an acceptor band:

A p-type semi-conductor

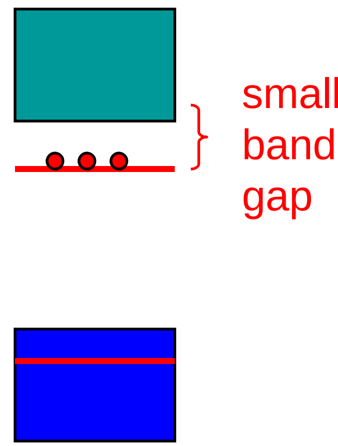
How Defects Improve Semi-Conduction

Pure Germanium



$\Delta E = 0.66$ eV

Arsenic-Doped Ge



As is more Electronegative:

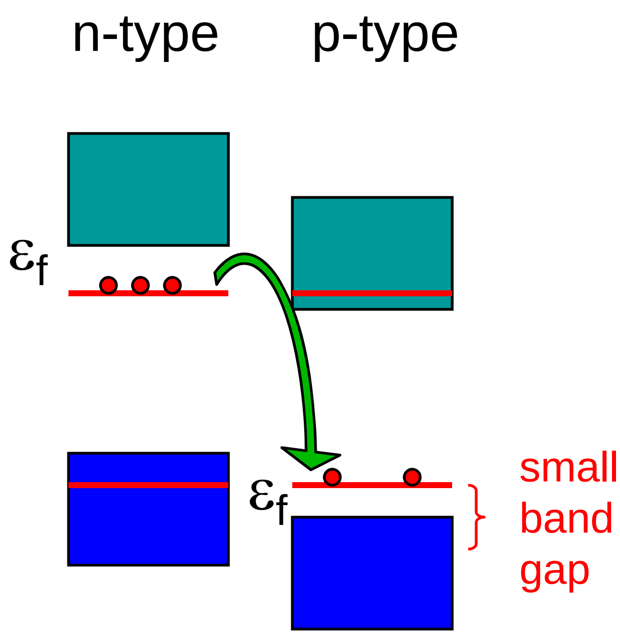
Adds “Orbitals” At Lower Energy Partially Filled with Electrons

Arsenic-Doping creates negative holes, as a donor band

An n-type semi-conductor

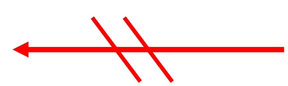
How Defects Lead to Devices

PN Junctions = Diodes



Fermi level in n-type semi-conductor is at higher energy than for the p-type:

Spontaneous flow of electrons in one direction only.



Directional Flow of electrons -->

current goes in one direction only

In a pn junction, current spontaneously flows in one direction