Linear Combination of Atomic Orbitals (LCAO)
Form Molecular Orbitals (MO) = Hybridization

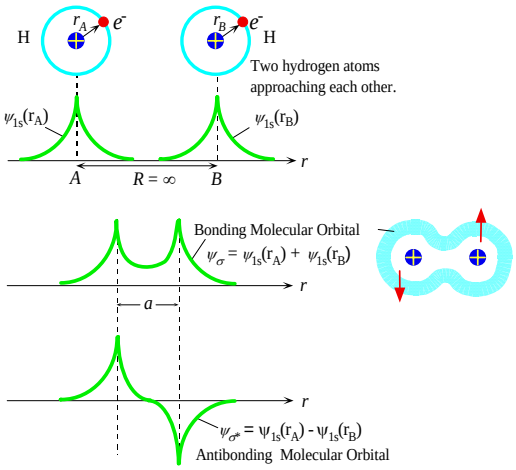

Fig. 4.1: Formation of molecular orbitals, bonding and antibonding (ψ_σ and ψ_{σ^*}) when two H atoms approach each other. The two electrons pair their spins and occupy the bonding orbital ψ_σ.

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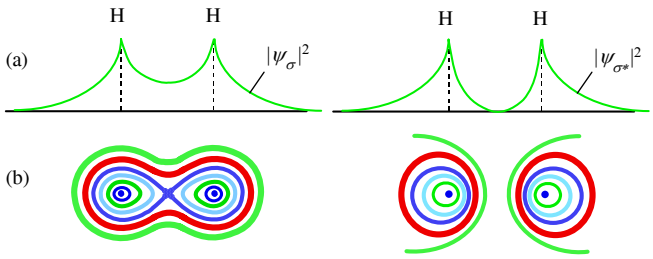

Fig. 4.2: (a) Electron probability distributions for bonding and antibonding orbitals, ψ_σ and ψ_{σ^*}. (b) Lines represent contors of constant probability (darker lines represent greater relative probability).

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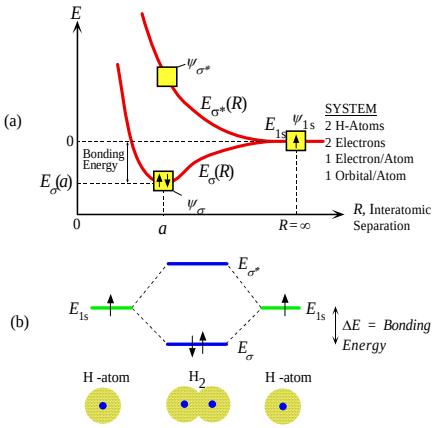

Fig. 4.3: Electron energy in the system comprising two hydrogen atoms. (a) Energy of ψ_σ and $\psi_{\sigma*}$ vs. the interatomic separation, R. (b) Schematic diagram showing the changes in the electron energy as two isolated H atoms, far left and far right, come to form a hydrogen molecule.

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HF – SP Hybridization

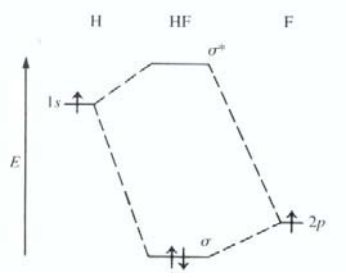

Figure 9.42
A partial molecular orbital energy-level diagram for the HF molecule. The bonding can be accounted for in terms of MOs formed from a fluorine 2p and a hydrogen 1s orbital. Note that bonding occurs because the two electrons have lower energy in the HF molecule than they do in the free hydrogen and fluorine atoms.

S. Zuhmdahl, **Chemistry** (Heath & Co., 1986)

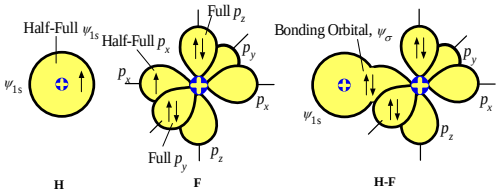

Fig. 4.6: H has one half empty ψ_{1s} orbital. F has one half empty p_x orbital but full p_y and p_z orbitals. The overlap between ψ_{1s} and p_x produces a bonding orbital and an antibonding orbital. The two electrons fill the bonding orbital and thereby form a covalent bond between H and F.

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Isolated Silicon

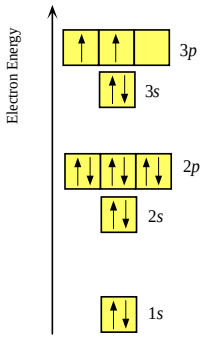

Fig. 4.15: The electronic structure of Si.

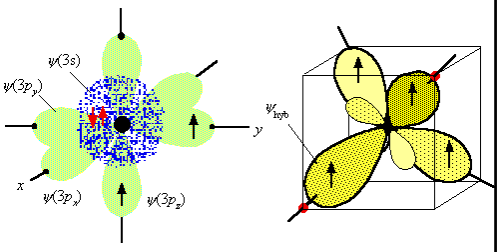

Fig. 4.16: (a). Si is in Group IV in the Periodic Table. An isolated Si atom has 2 electrons in the 3*s* and 2 electrons in the 3*p* orbitals. (b) When Si is about to bond, the *one* 3*s*-orbital and the *three* 3*p*-orbitals become perturbed and mixed to form four hybridized orbitals, ψ_{hyb}, called sp^3 orbitals which are directed towards the corners of a tetrahedron. The ψ_{hyb} orbital has a large major lobe and a small back lobe. Each ψ_{hyb} orbital takes one of the four valence electrons.

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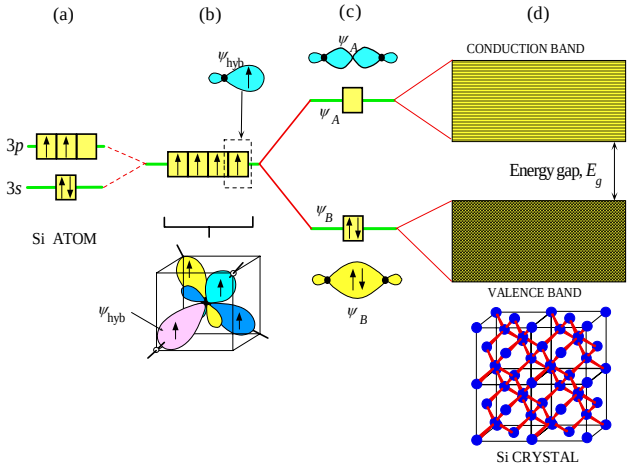

Fig. 4.17: (a) Formation of energy bands in the Si crystal first involves hybridization of 3*s* and 3*p* orbitals to four identical ψ_{hyb} orbitals which make 109.5° with each other as shown in (b). (c) ψ_{hyb} orbitals on two neighboring Si atoms can overlap to form ψ_B or ψ_A. The first is a bonding orbital (full) and the second is an antibondiong orbital (empty). In the crystal ψ_B overlap to give the valence band (full) and ψ_A overlap to give the conduction band (empty).

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TiO_2

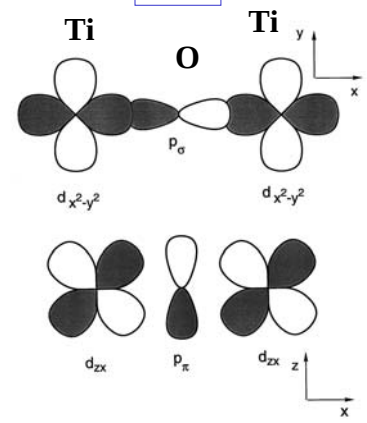
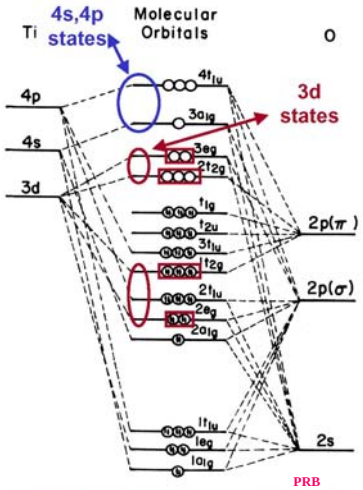


FIG. 3. Examples of configurations for transition-metal $3d$ orbitals which are bridged by ligand p orbitals.

Imada *et al.*, Review of Modern Physics (1998)



*Ref. 16 in LA Grunes, PR 27, 2111 (1983)

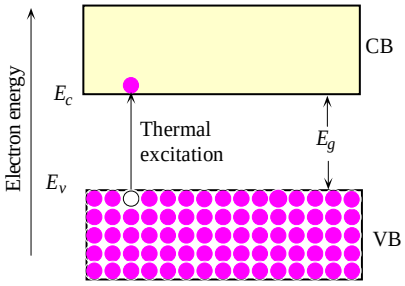


Fig. 4.18: Energy band diagram of a semiconductor. CB is the conduction band and VB is the valence band. At 0 K, the VB is full with all the valence electrons.

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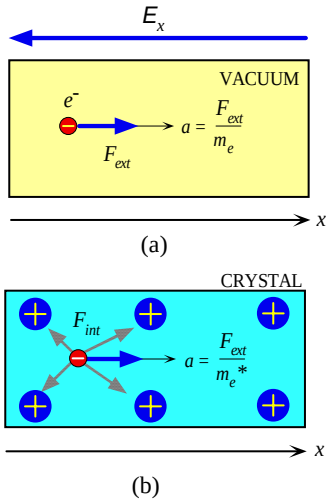

Fig. 4.19: (a) An external force F_{ext} applied to an electron in vacuum results in an acceleration $a_{vac} = F_{ext} / m_e$. (b) An external force F_{ext} applied to an electron in a crystal results in an acceleration $a_{cryst} = F_{ext} / m_e^*$. ($E_x$ is the electric field.)

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