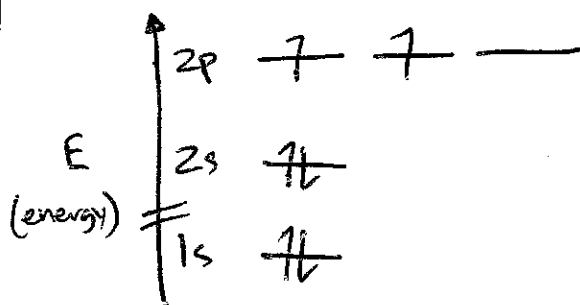


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Course website: www.chem.wisc.edu/chem343-hackenberger

recall:

- Carbon: 4 valence electrons
- Orbitals: 3D-space in which e^- can be found
- 4 valence e^- can be found in 4 atomic orbitals (AO)
 - carbon: $2s, 2p_x, 2p_y, 2p_z$ (read p. 23)
- 2 situations: e^- in AO's, and e^- in molecular orbitals (MO's)

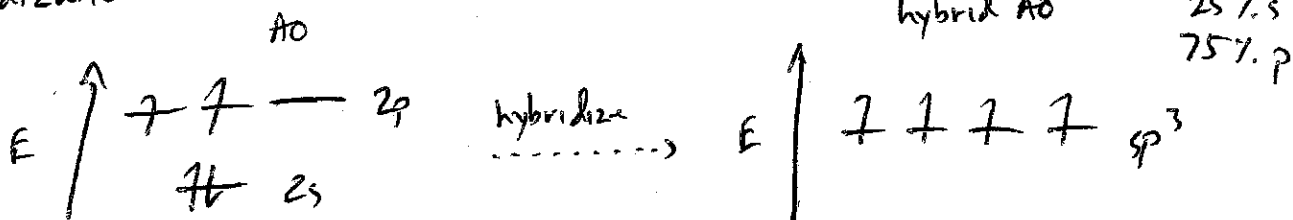


Aufbau principle

Pauli: no two electrons in an orbital can have the same quantum # (must have different spins $\uparrow\downarrow$)

Hund: First, place e^- in orbitals of equal E
 Second, spins are in the same direction when comparing e^- at same energy level

• Hybridization

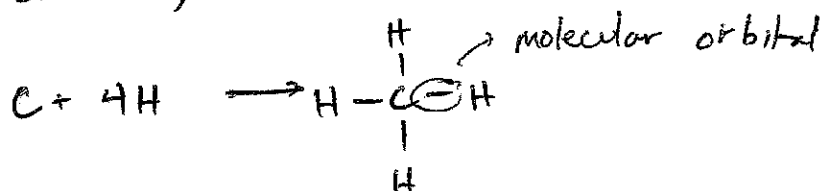


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• Hybridization: Schrodinger: LCAO (Linear combination of AO)

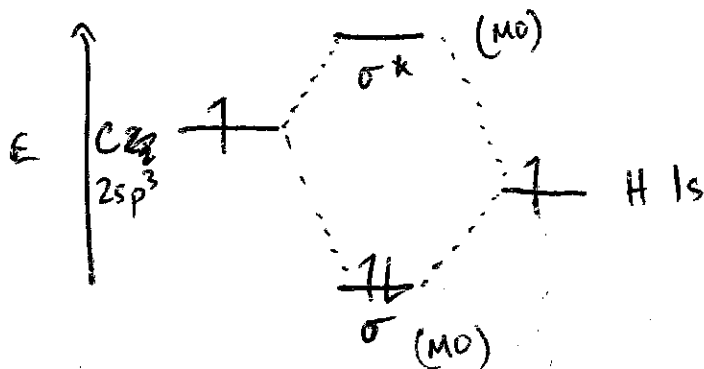
• The structural consequence of hybridization is that the 4 sp^3 orbitals have a tetrahedral geometry

• Prototypical organic molecule: Methane CH_4



• How can we describe a MO?

1) Energy diagram



In energetic ground state, σ is filled

• Roman letters for AO

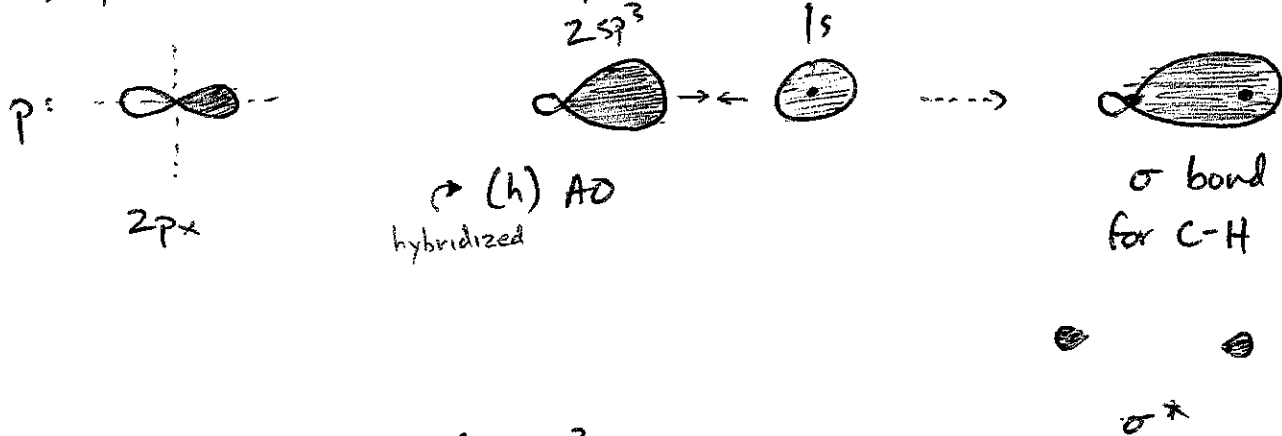
• Greek letters for MO

• Same number of AO's and MO's (2 each here)

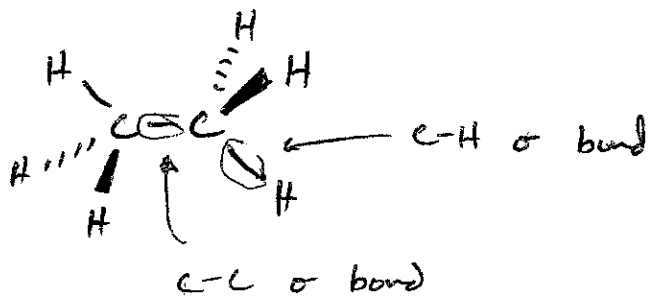
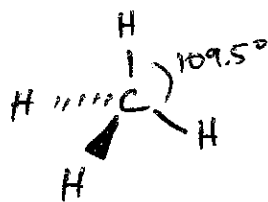
• σ is lower energy than AO's, σ^* is higher

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2) Spatial characteristics (p. 39)



• 3D perspective drawing for sp^3 carbon



• Ethane, C_2H_6