Bonding in Organic Molecules and Reactivity

- ✓ Valence Bond Theory (VBT): Resonance, Hybridization
- ✓ Molecular Orbital Theory (MOT): Molecular orbitals

- ➢ Organic chemists like to use the concept of hybridization and resonance whenever possible
- ➢ Molecular Orbital Theory is more sophisticated and more precise
- ➢ However, *in many instances a better picture of bonding is described by combining the hybrid approach with delocalized MO approach*

Course Content for my part

- ✓ Hybrid Atomic Orbitals (VBT)
- ✓ Conjugation and Delocalization (VBT / MOT)
- ✓ Molecular Orbitals and Organic Reactions

  S_N1 and **S_N2**

Study Material

First 3 classes: Mostly from Keeler-Wothers, 2nd Edition (Chapter 5)

- **Page 164 to 176**

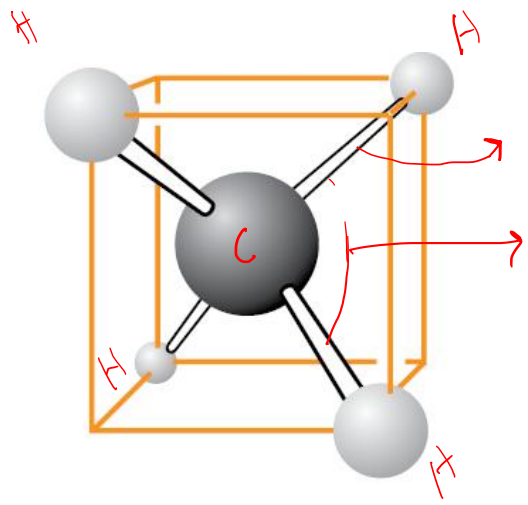
Hybrid Atomic Orbitals

✓ As CH_4 is tetrahedral, we should construct some new orbitals on the carbon that point towards the corners of a tetrahedron

✓ The important thing is that were combing the AOs from the same atom, in contrast to when MOs are formed where we combine AOs from different atoms

C: $2s^2\ 2p^2$ ↓ HAO

$4SP^3$



a molecule of methane enclosed in a cube

CH_4

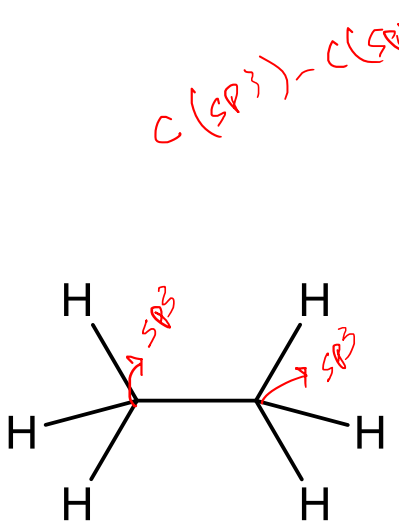
1.09 Å

109.5°

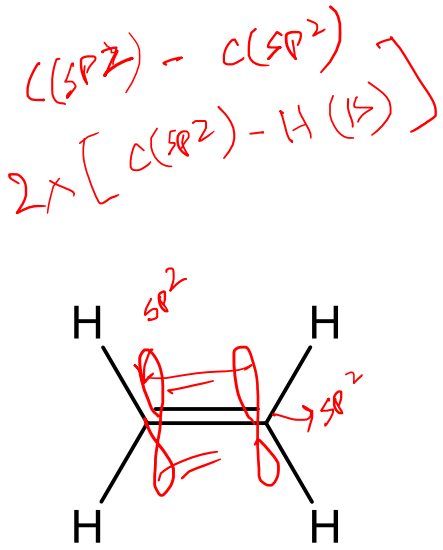
$4 \times [C(SP^3) : H(1S)]$ ↓ $4 \times C-H$ (σ)

Bonding In Organic Molecules

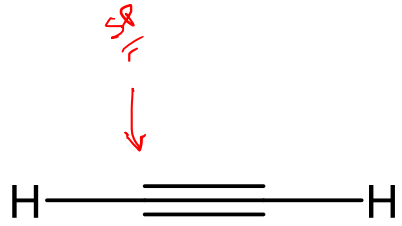
- ✓ Hybrid orbitals to describe the bonding in organic molecules
- ✓ In reactions, the form of HOMO and LUMO are quite important (we will see later)



Ethane

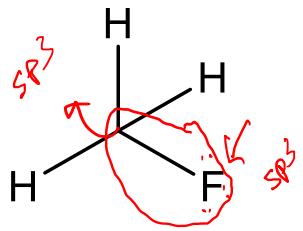


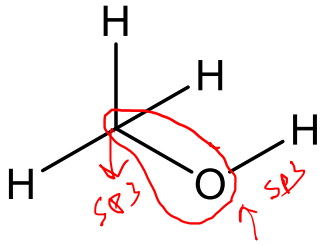
Ethylene

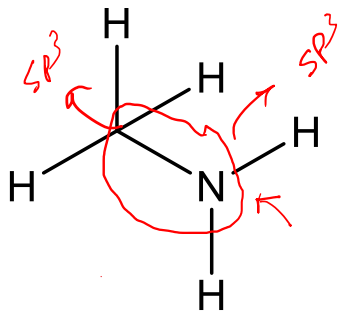


Acetylene

Halides, Alcohols and Amines

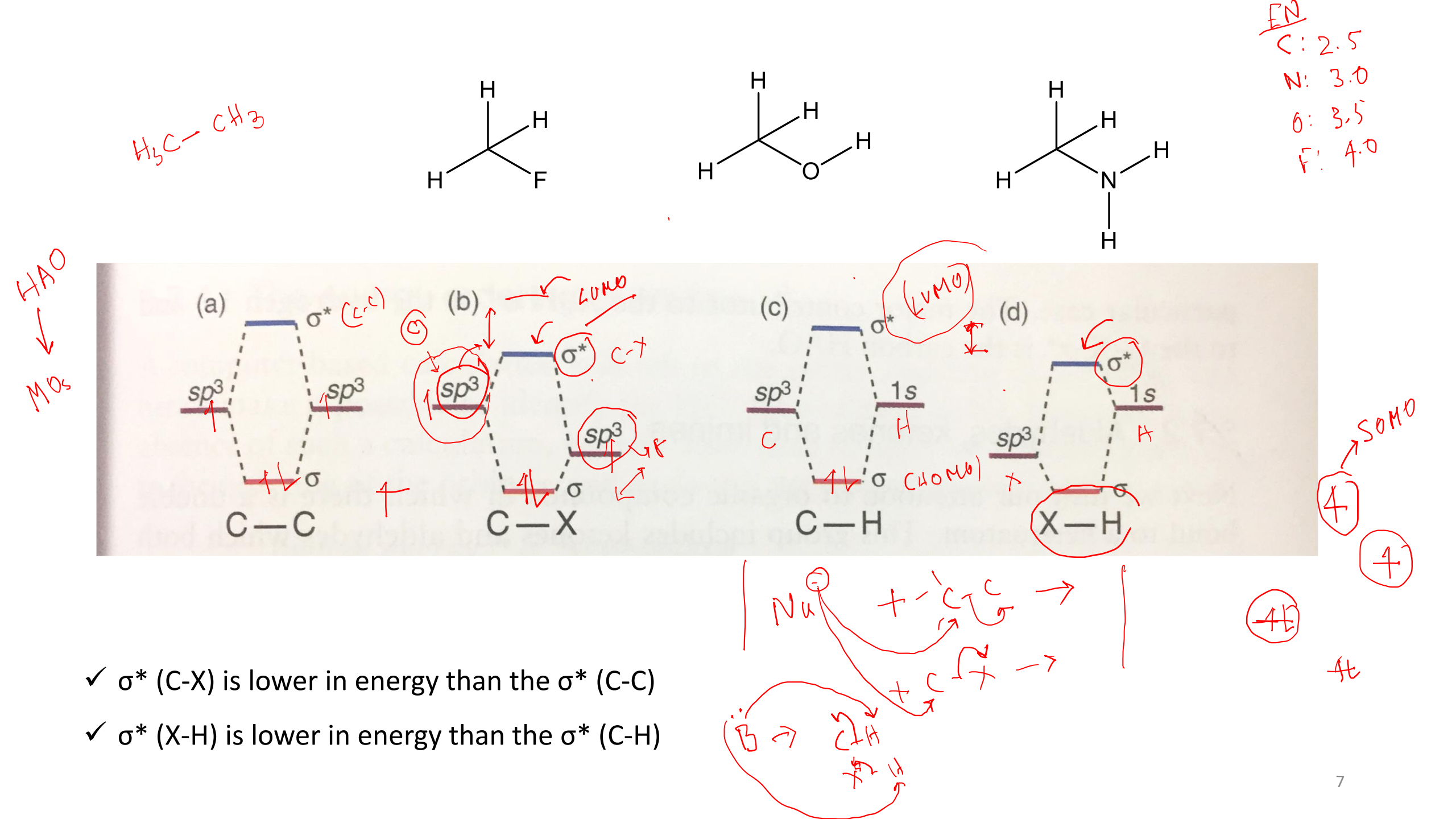






- ✓ CH_3F, CH_3OH and CH_3NH_2: 3 very common organic molecules
- ✓ The arrangement of atoms around the carbon is close to tetrahedral: sp^3 hybridized
- ✓ We will also assume the heteroatom (F, O and N) are also sp^3 hybridized

- ✓ In all the molecules, the HOMO is essentially one of the heteroatom hybrid atomic orbitals not involved in bonding
- ✓ LUMO are σ* antibonding MOs associated with C-H, X-H and C-X bonds.



- ✓ σ* (C-X) is lower in energy than the σ* (C-C)
- ✓ σ* (X-H) is lower in energy than the σ* (C-H)