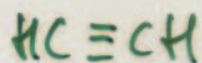


# s-p hibridpályák

**sp** (lineáris)



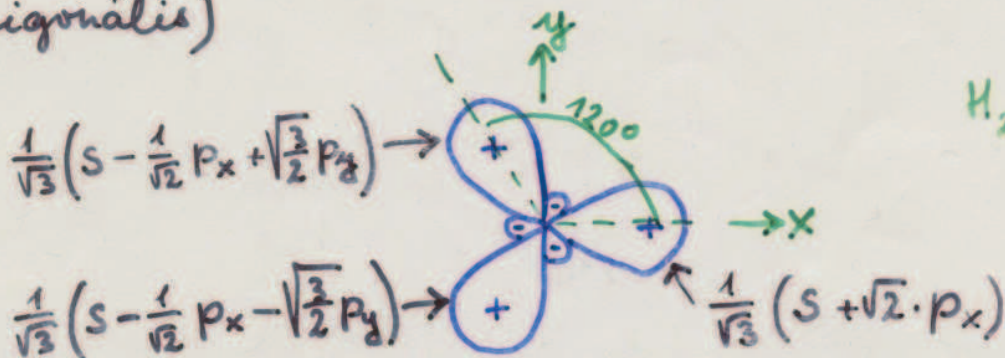
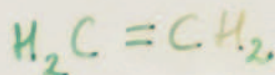
$$\frac{1}{\sqrt{2}}(s + p_z)$$



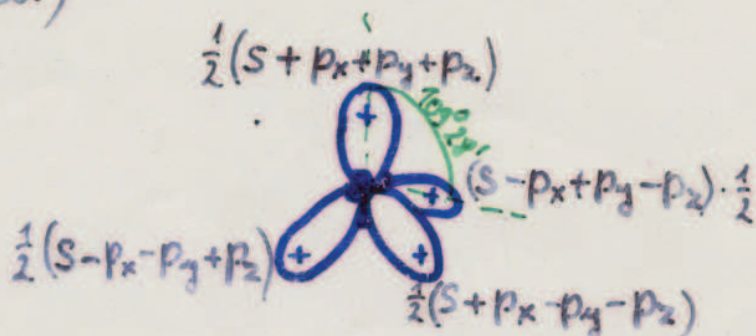
$$\frac{1}{\sqrt{2}}(s - p_z)$$

→ 2

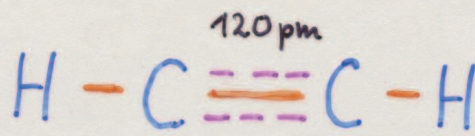
**sp<sup>2</sup>** (trigonális)



**sp<sup>3</sup>** (tetragonális)

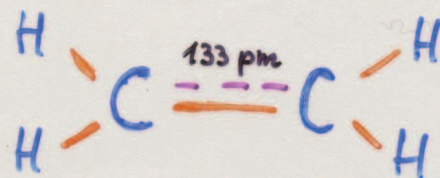


$sp^1$  (lineáris) :



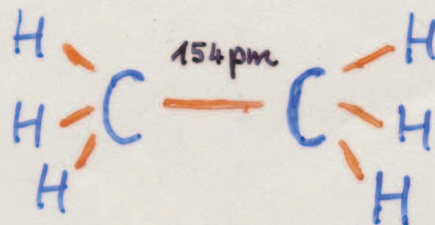
acetilén

$sp^2$  (trigonális) :



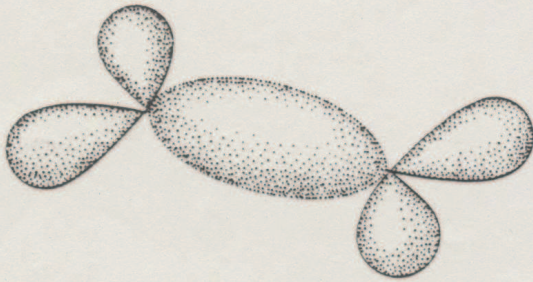
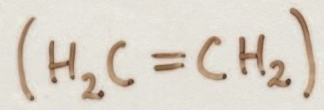
etilén

$sp^3$  (tetragonális) :

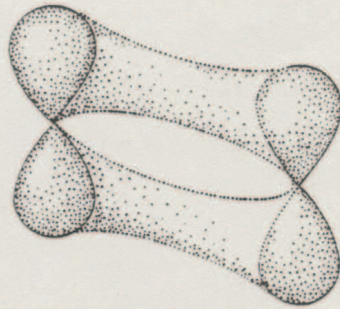


etán

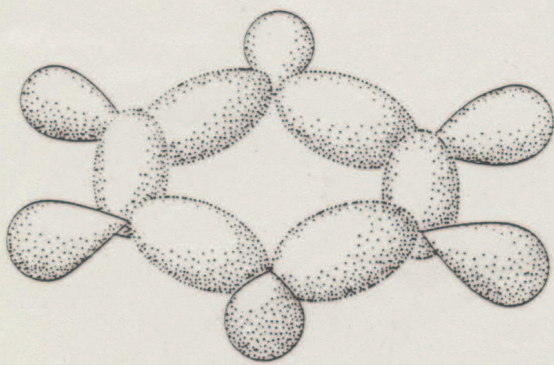
etilén



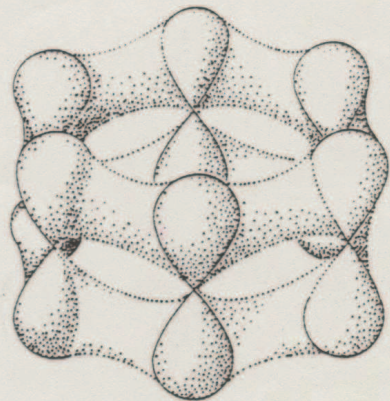
$\sigma$



$\pi$

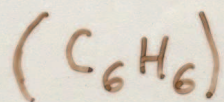


$\sigma$



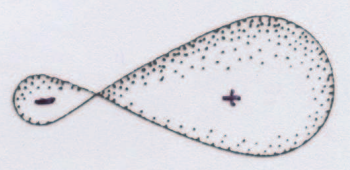
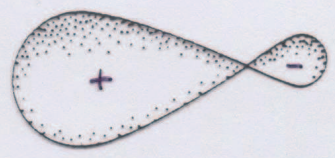
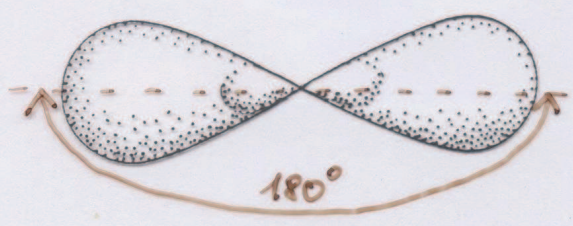
$\pi$

benzol

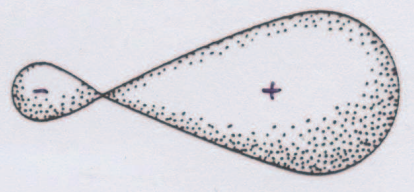
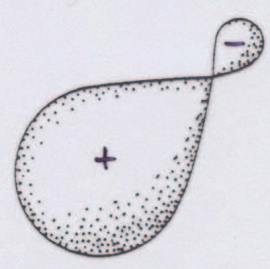
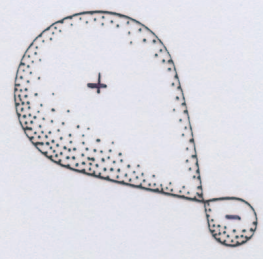
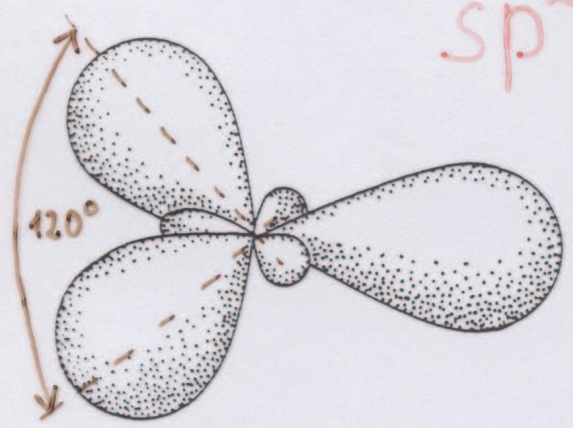


sp - hibridpályák

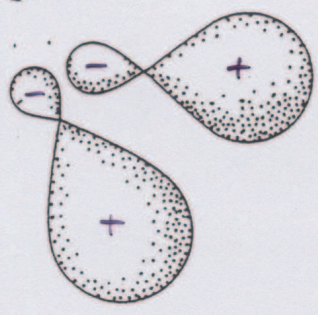
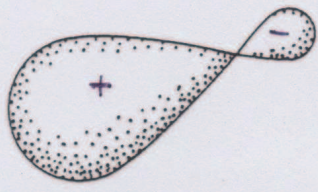
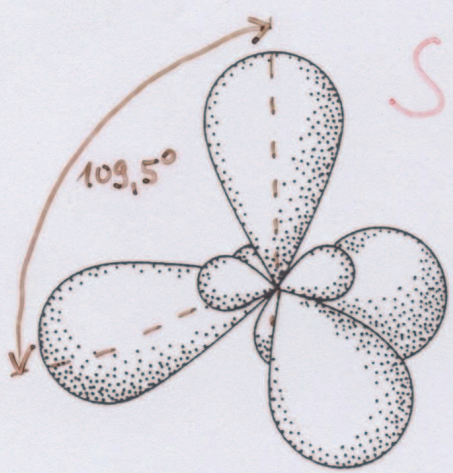
sp<sup>1</sup>



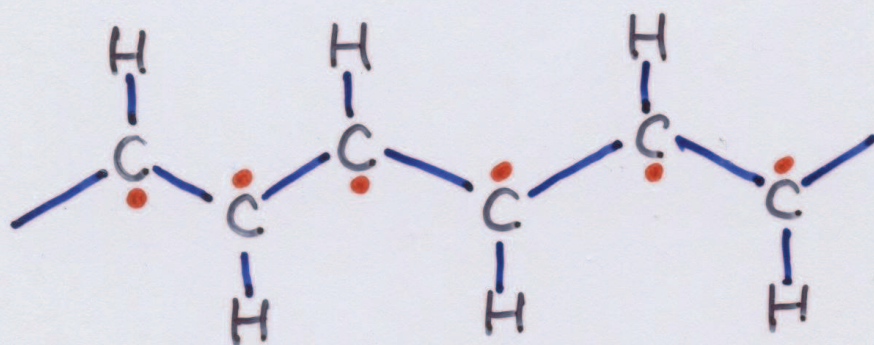
sp<sup>2</sup>



sp<sup>3</sup>



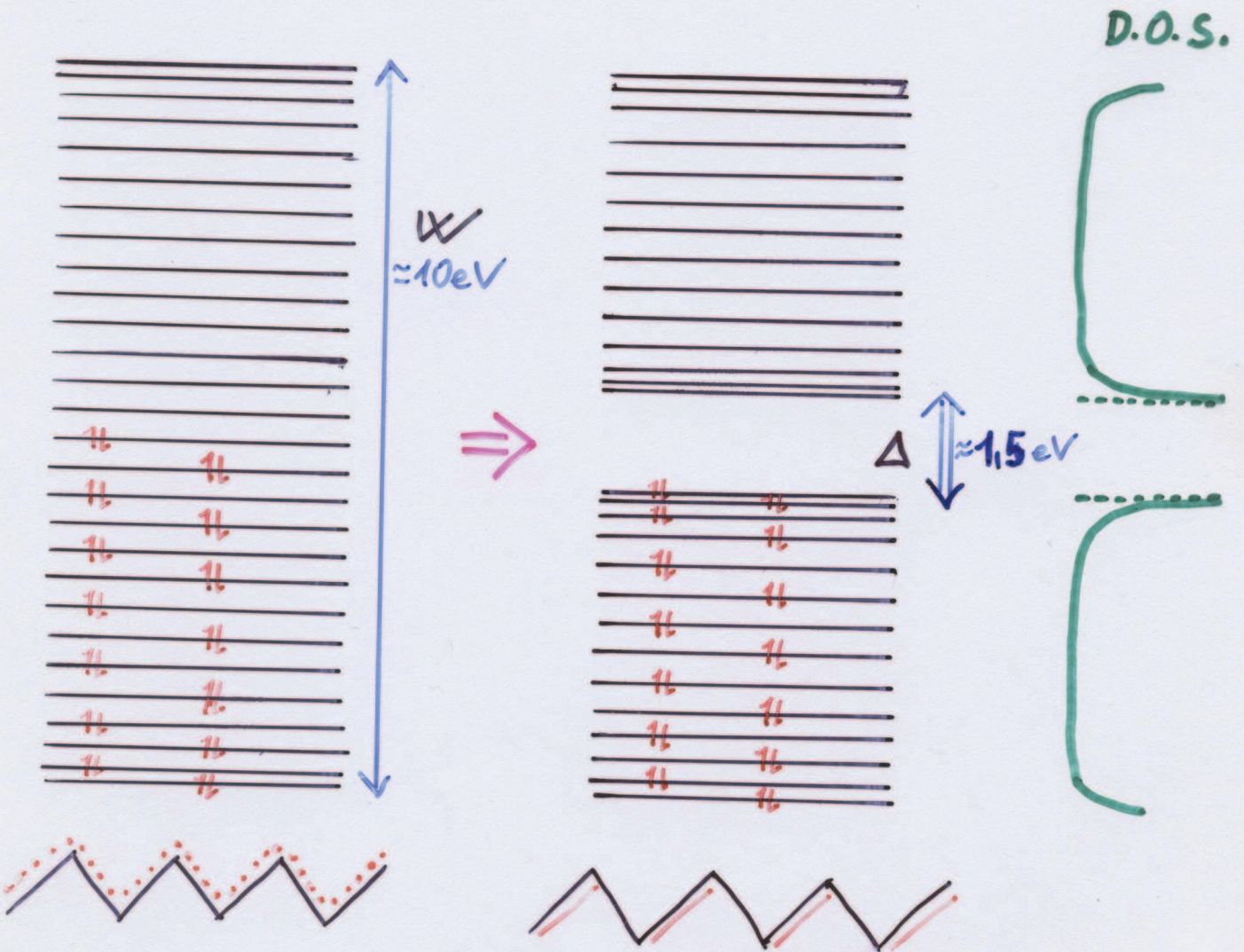
# trans - POLYACETYLENE



$sp^2$  hybrid orbital : 3 / carbon atom  
→  $\sigma$ -band, fully occupied

$p_z$  orbital : 1 / carbon atom  
→  $\pi$ -band, half filled

# trans - PA

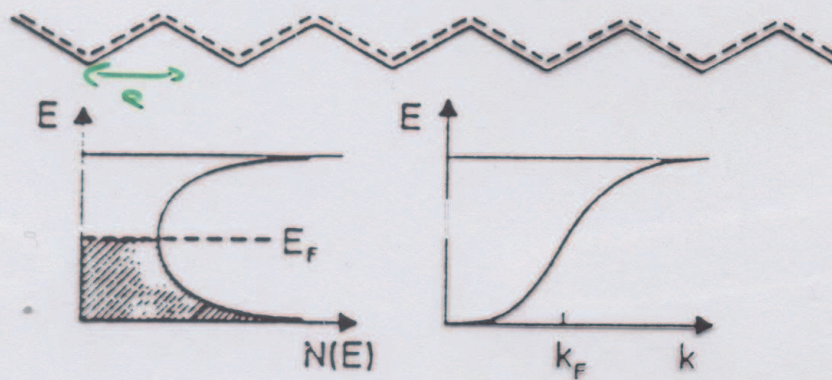


$$\pi_{\parallel} \approx 1,36 \text{ \AA}$$

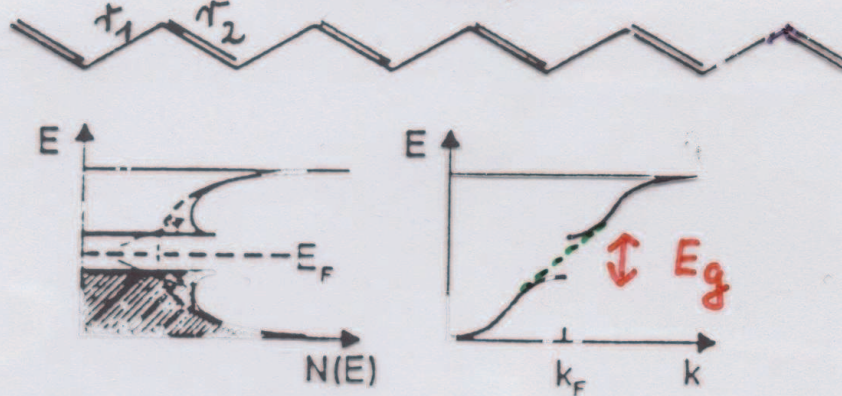
$$\pi_{\perp} \approx 1,44 \text{ \AA}$$

# Peierls instability in 1D

metallischer Zustand



Isolatorzustand

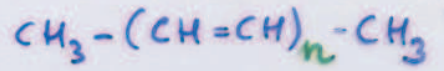
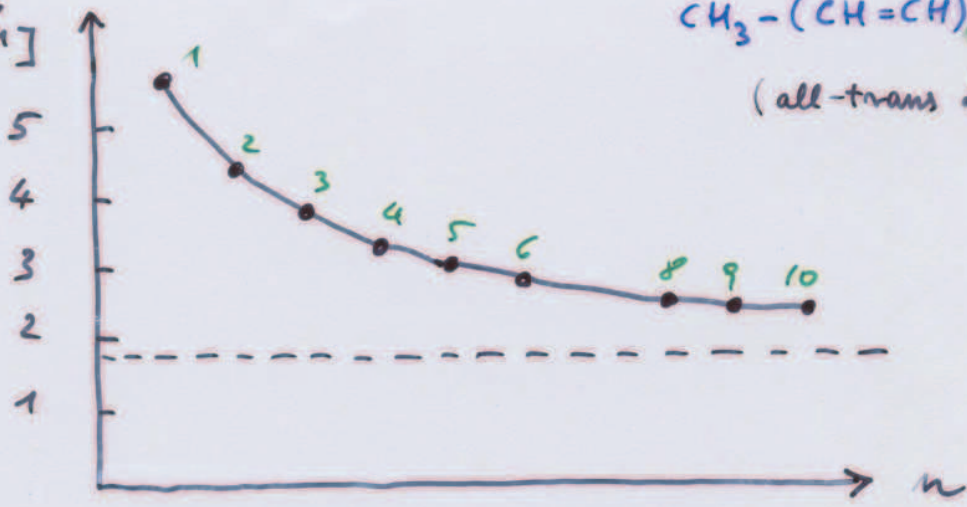


$$\Delta\tau = \tau_1 - \tau_2$$

$$\underline{E_g \sim \Delta\tau}$$

i) gap

$\nu_{max}$   
[ $10^4 \text{ cm}^{-1}$ ]

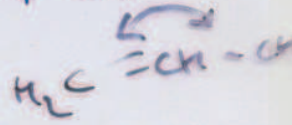


(all-trans  $\omega, \omega'$  dimethylpolyene)

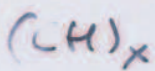
"dibondok szint  
négyesek"  
 $\Delta E \sim \frac{1}{n}$

Konjugált polimerekben

$E_g \approx 1.5 - 4 \text{ eV}$



ii) alternálás

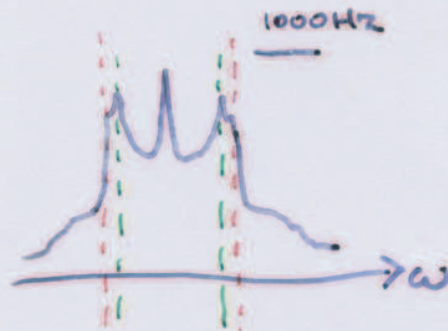
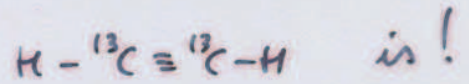


$^{13}\text{C}$  NMR

(Yannoni, Clark)

Előállításnál:

kevés



$\Rightarrow \tau_1 \approx 1.44 \text{ \AA}$   
 $\tau_2 \approx 1.36 \text{ \AA}$

Félszázados dipól-dipól kkv. miatt