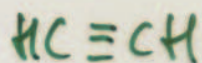


s-p hibridpályák

sp (lineáris)



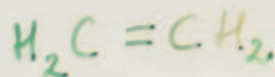
$$\frac{1}{\sqrt{2}}(s + p_z)$$



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

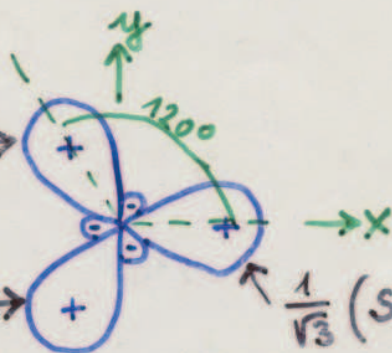
→ z

sp² (trigonális)



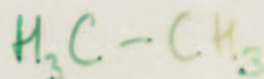
$$\frac{1}{\sqrt{3}}\left(s - \frac{1}{\sqrt{2}}p_x + \sqrt{\frac{3}{2}}p_y\right)$$

$$\frac{1}{\sqrt{3}}\left(s - \frac{1}{\sqrt{2}}p_x - \sqrt{\frac{3}{2}}p_y\right)$$

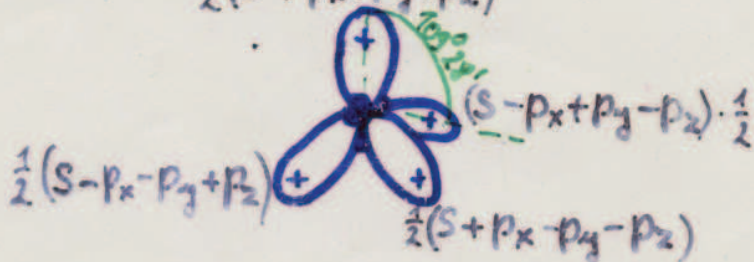


$$\frac{1}{\sqrt{3}}(s + \sqrt{2} \cdot p_x)$$

sp³ (tetragonális)

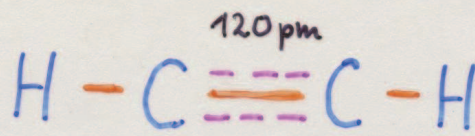


$$\frac{1}{2}(s + p_x + p_y + p_z)$$



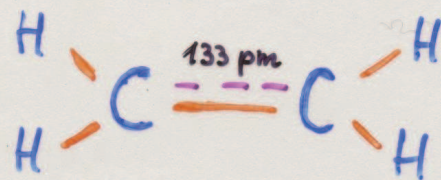
$$\frac{1}{2}(s + p_x - p_y - p_z)$$

sp^1 (lineáris) :



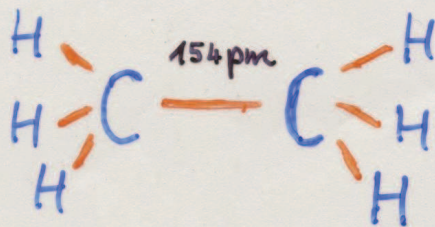
acetilén

sp^2 (trigonális) :



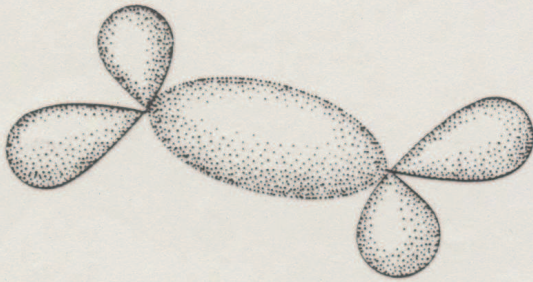
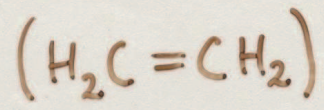
etilén

sp^3 (tetragonális) :

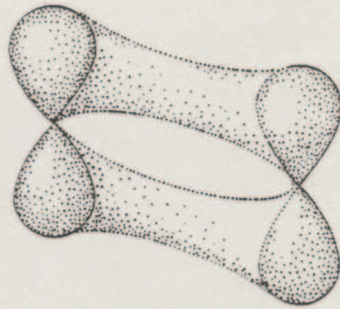


etán

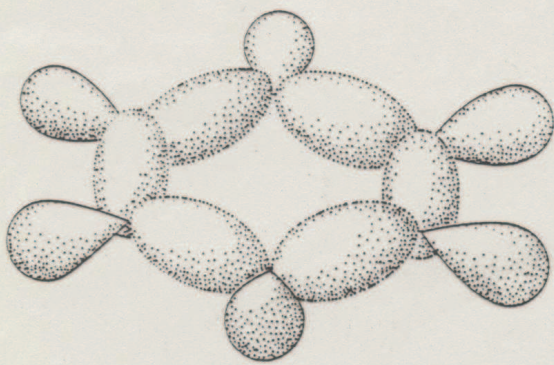
etilén



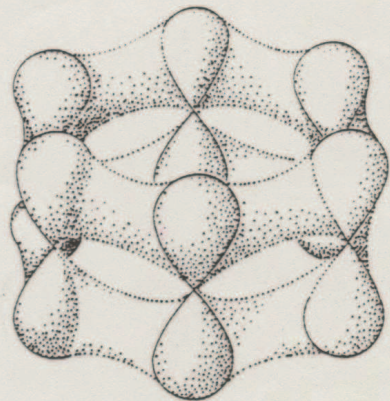
σ



π

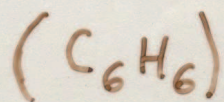


σ



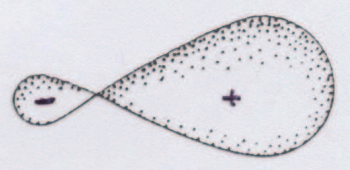
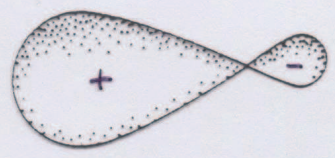
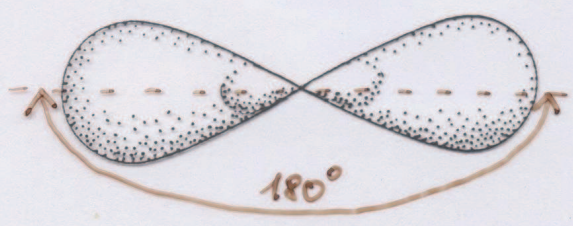
π

benzol

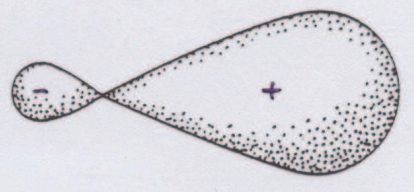
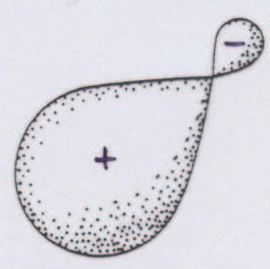
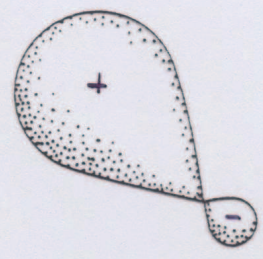
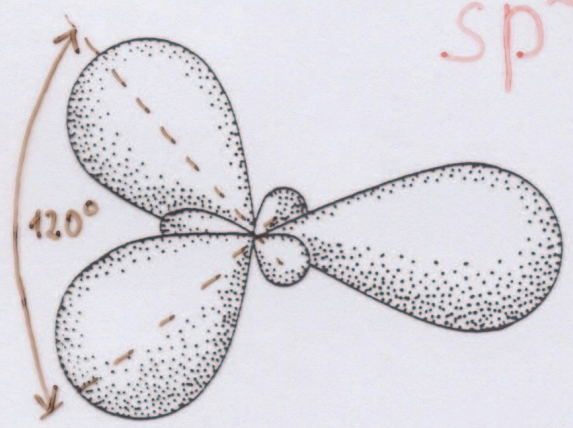


sp - hibridpályák

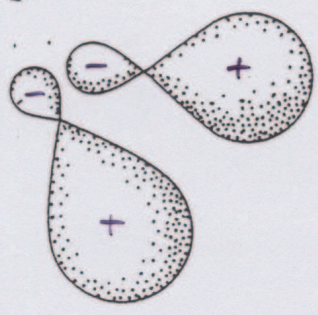
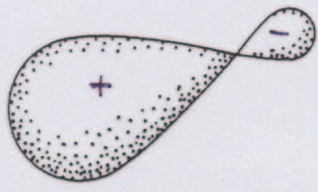
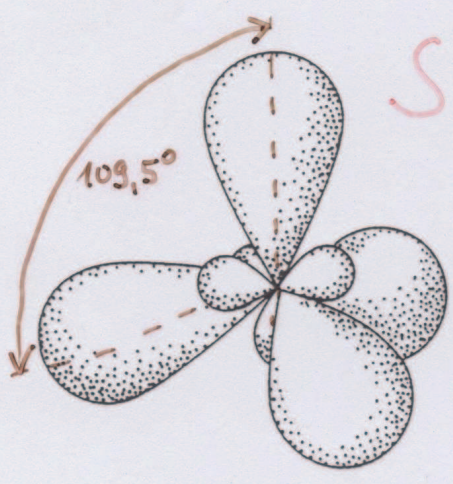
sp¹



sp²



sp³



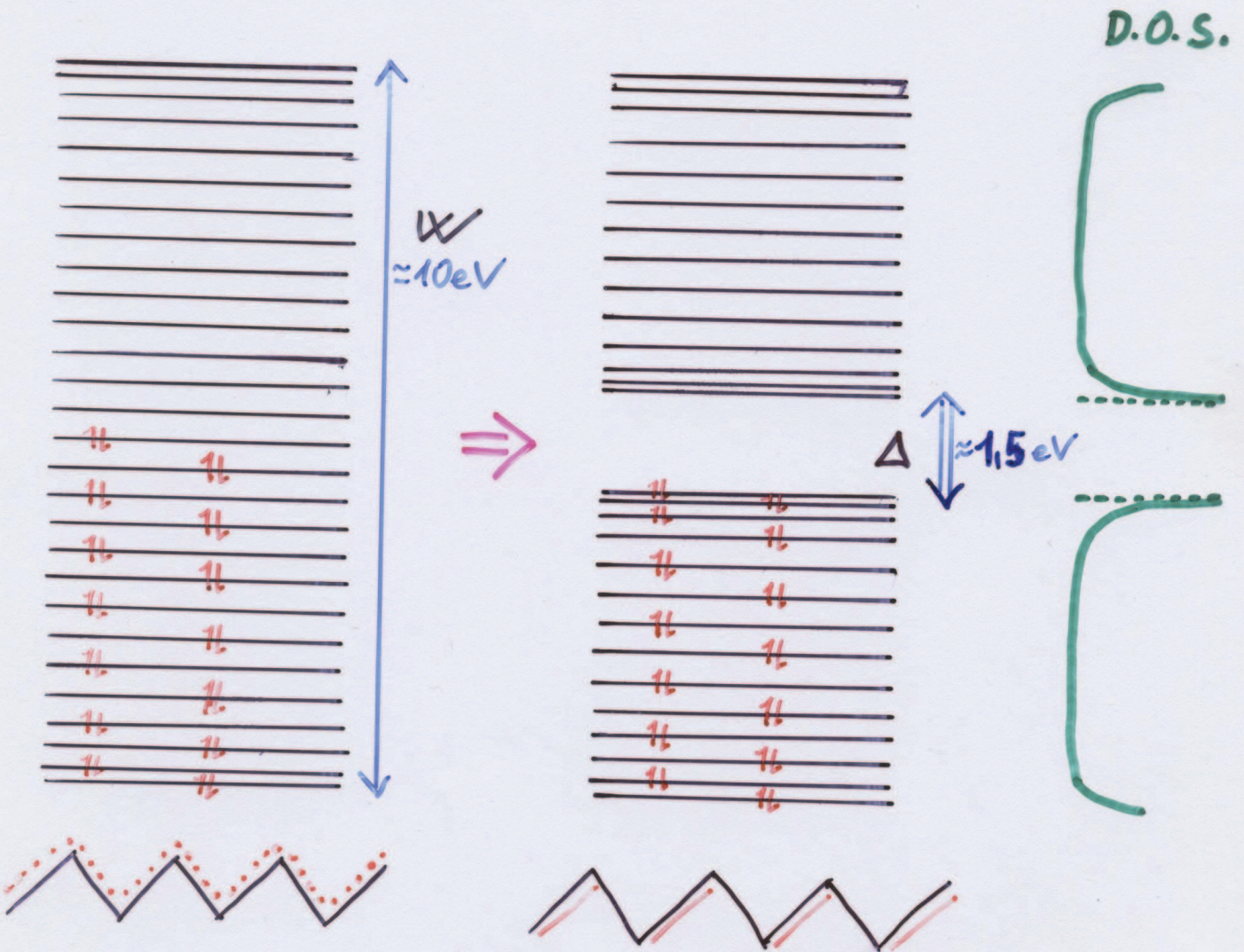
trans - POLYACETYLENE



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

p_z orbital : 1 / carbon atom
→ π -band, half filled

trans - PA

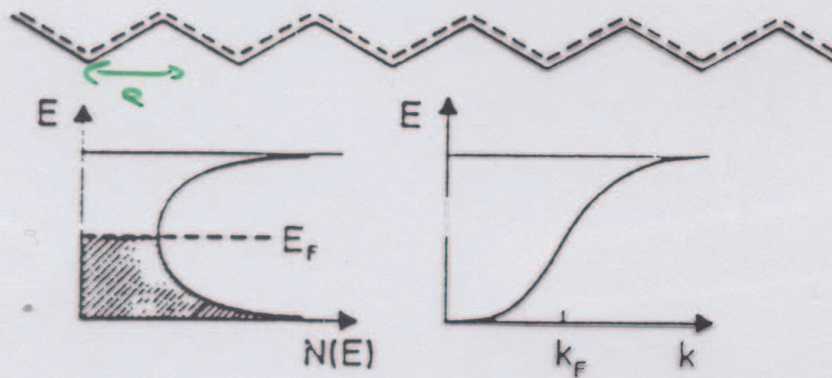


$$\pi_{\parallel} \approx 1,36 \text{ \AA}$$

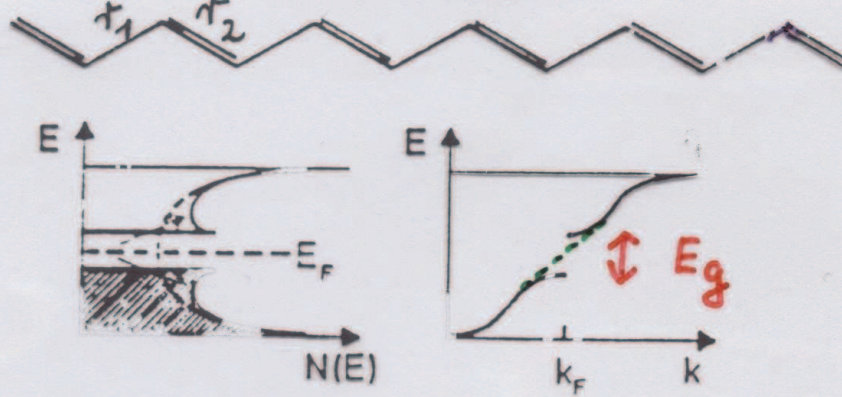
$$\pi_{\perp} \approx 1,44 \text{ \AA}$$

Peierls instability in 1D

metallischer Zustand



Isolatorzustand



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

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