

MACROMOLECULES

lecture for physics and biophysics students

2018. winter semester – 1. October

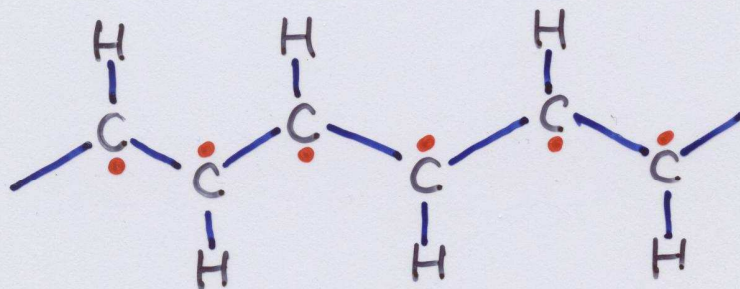
 **Jenő KÜRTI**

Eötvös Loránd University

Institute of Physics

Department of Biological Physics

trans - POLYACETYLENE



sp^2 hybrid orbital : 3 / carbon atom

→ σ -band, fully occupied

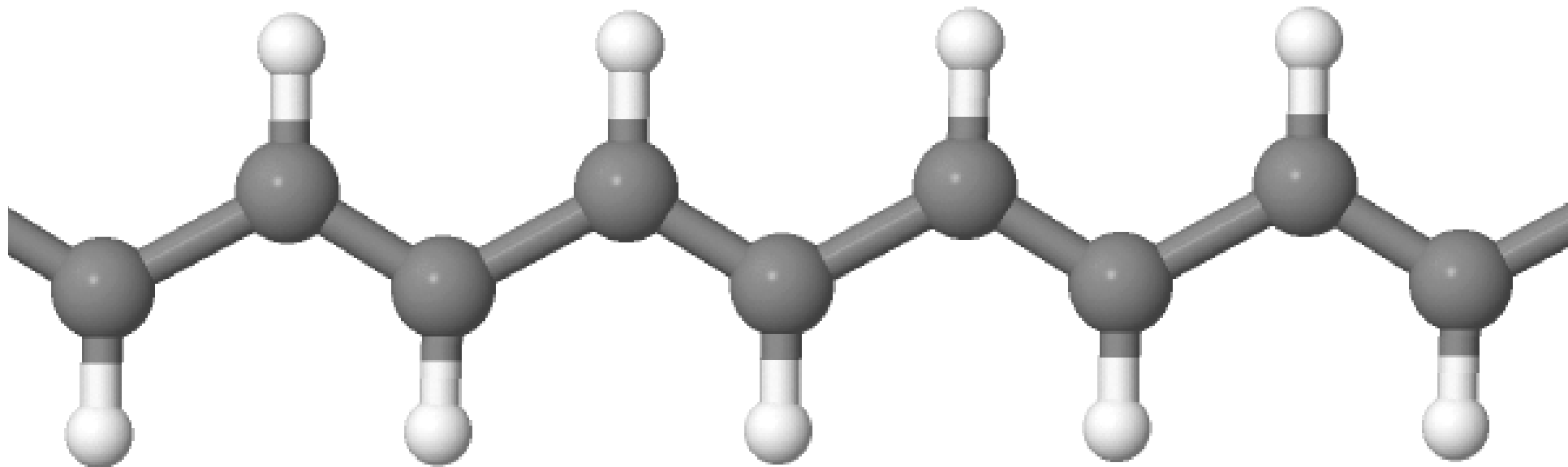
p_z orbital : 1 / carbon atom

→ π -band, half filled

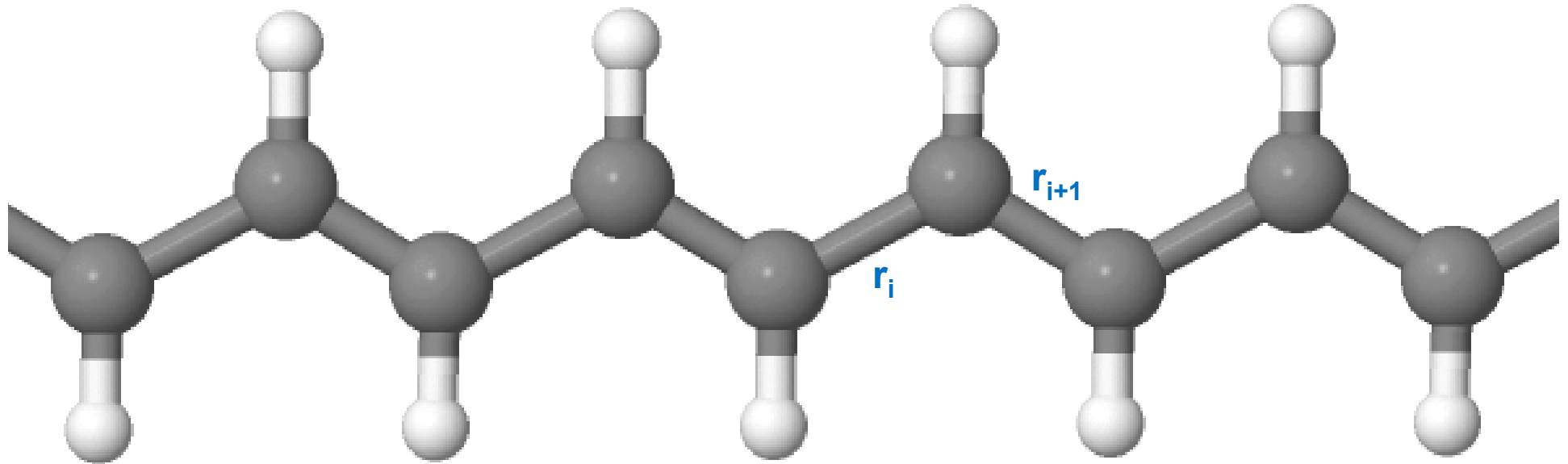
SÁVSZERKEZET:

σ

π

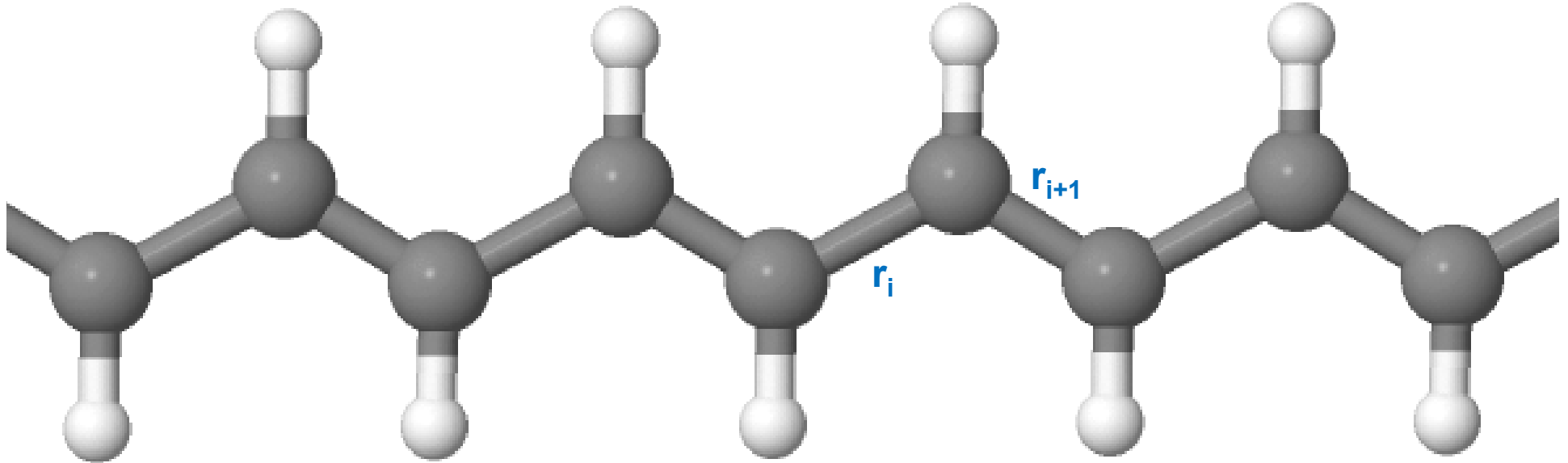


Bond Length Alternation: $BLA_i = |r_{i+1} - r_i|$



physics student : $BLA = 0$

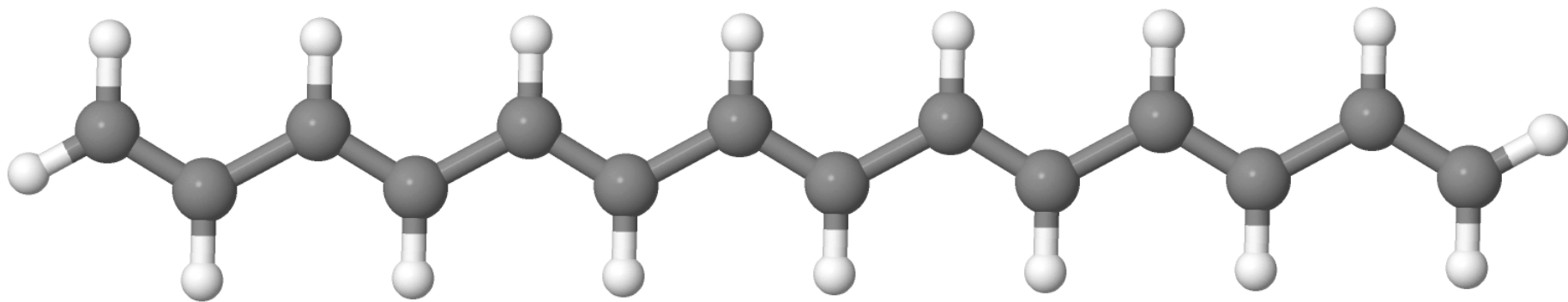
Bond Length Alternation: $BLA_i = |r_{i+1} - r_i|$



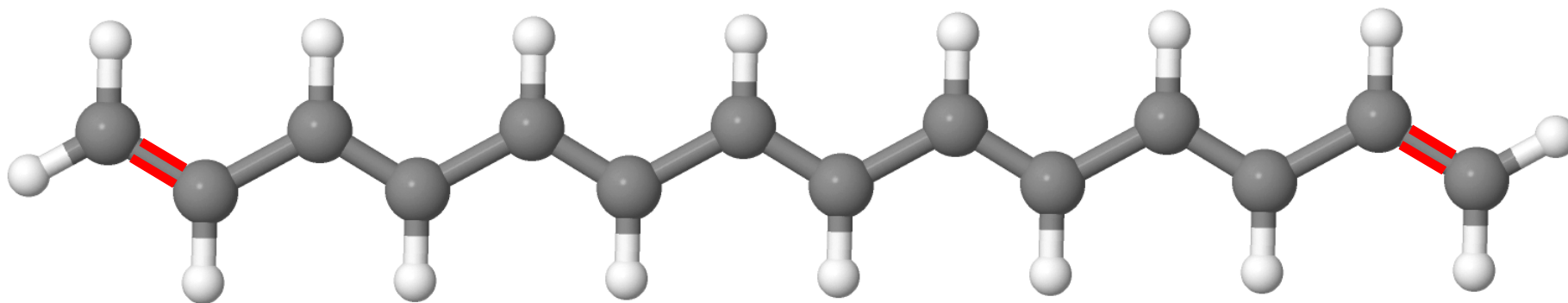
physics student : $BLA = 0$

chemistry student : $BLA = R_1 - R_2 \approx 21 \text{ pm}$

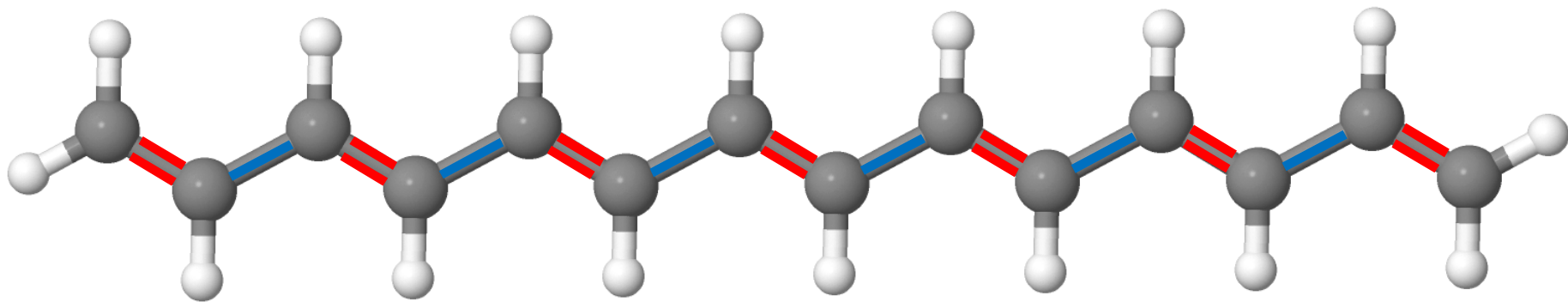
finite oligomer: chain end effects



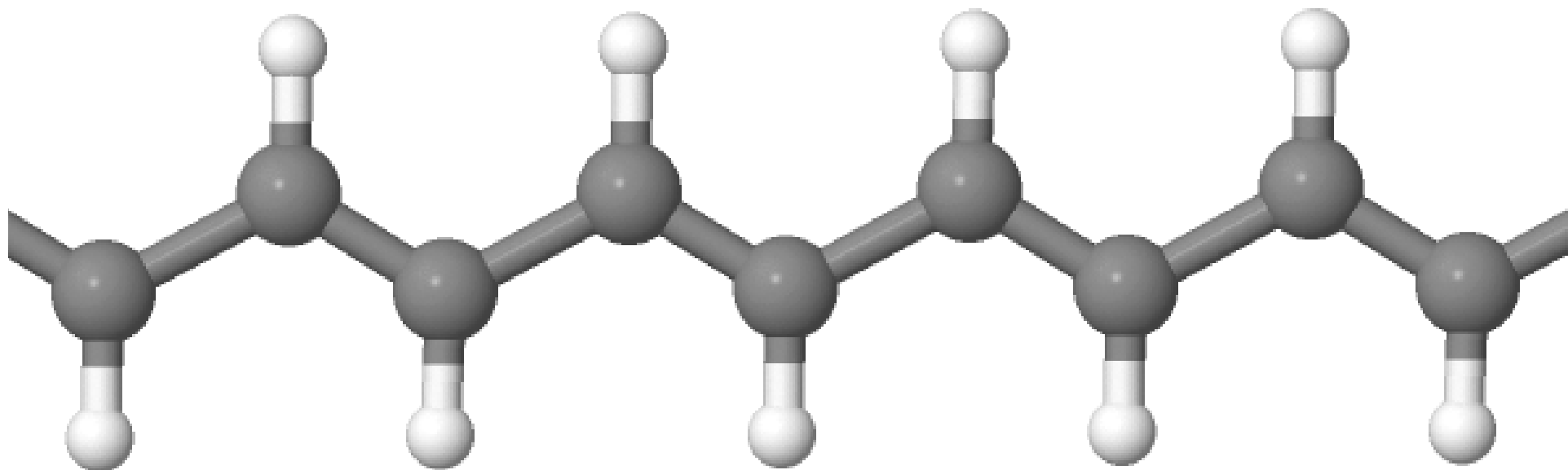
finite oligomer: chain end effects



finite oligomer: chain end effects

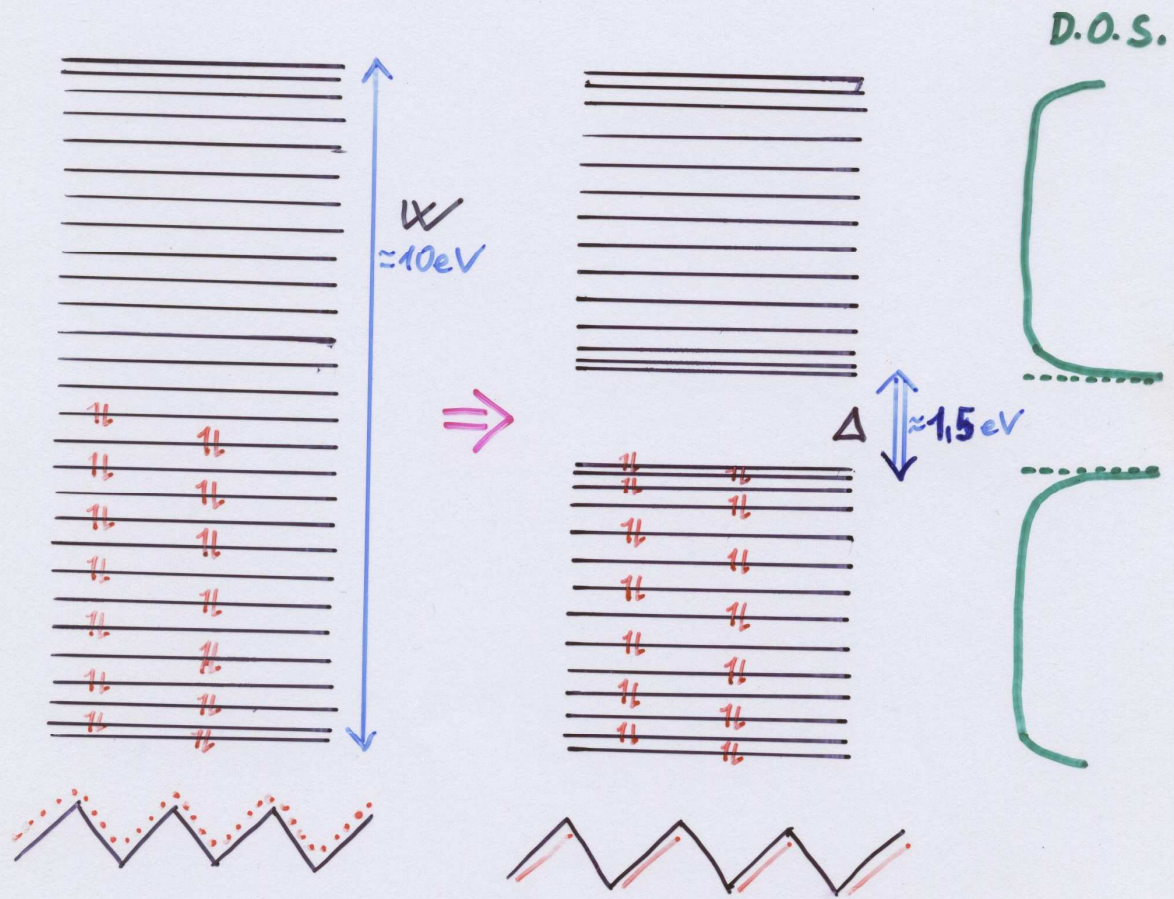


infinite polymer: ???



Móricka ábrák a molekulapályákról ...

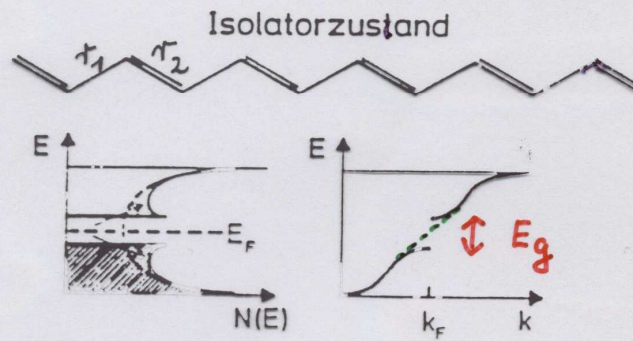
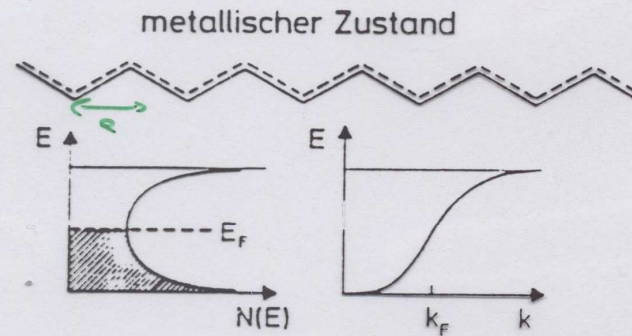
trans - PA



$$\tau_{||} \approx 1,36 \text{ \AA}$$

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

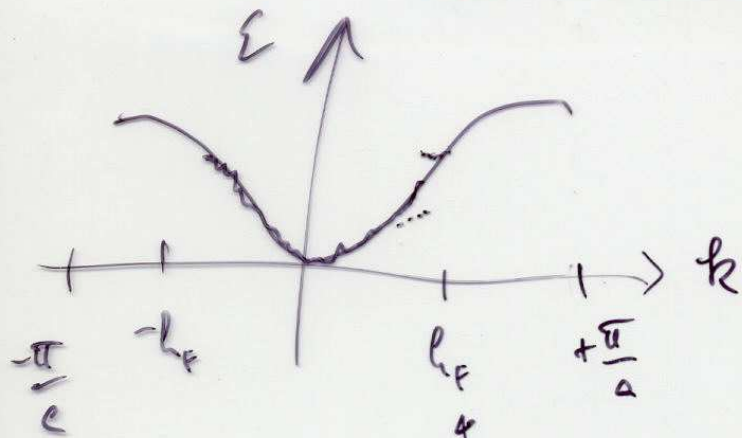
Peierls instability in 1D



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

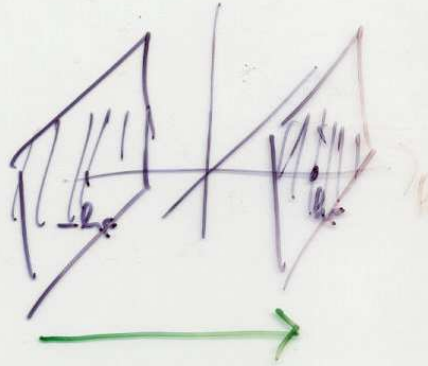
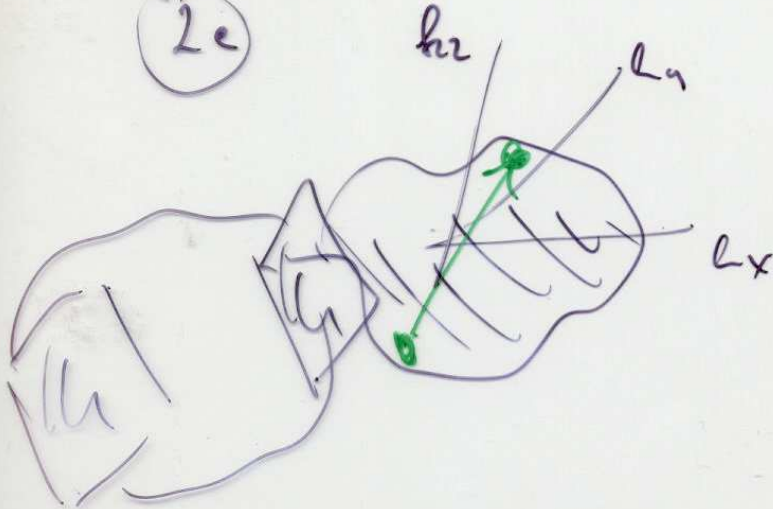
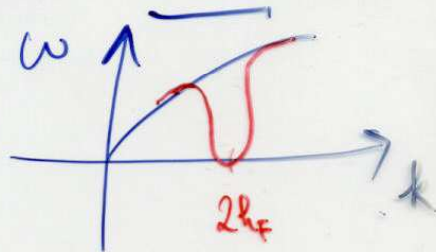
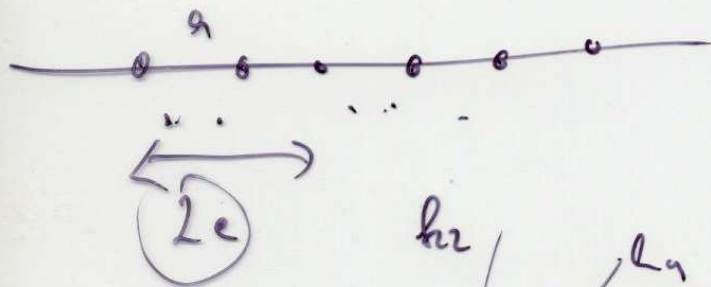
$$\underline{E_g \sim \Delta\tau}$$

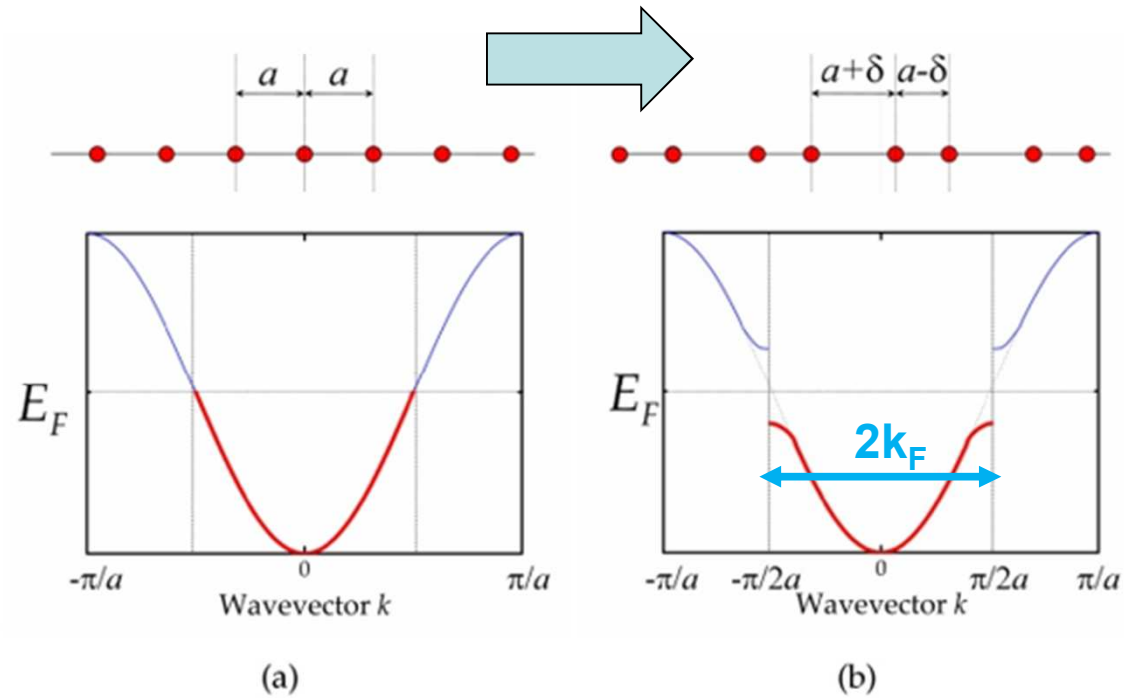
1dim instabilität



$$2k_F$$

$2k_F = \frac{\pi}{a} \approx \frac{2\pi}{2a}$
 Period \leftrightarrow Kohle





Peierls-instabilitás

(https://www.utwente.nl/tnw/pin/onderzoek/physical_properties_of_low-dimensional_systems/physical_properties_of_low-dimensional_systems-8.png)