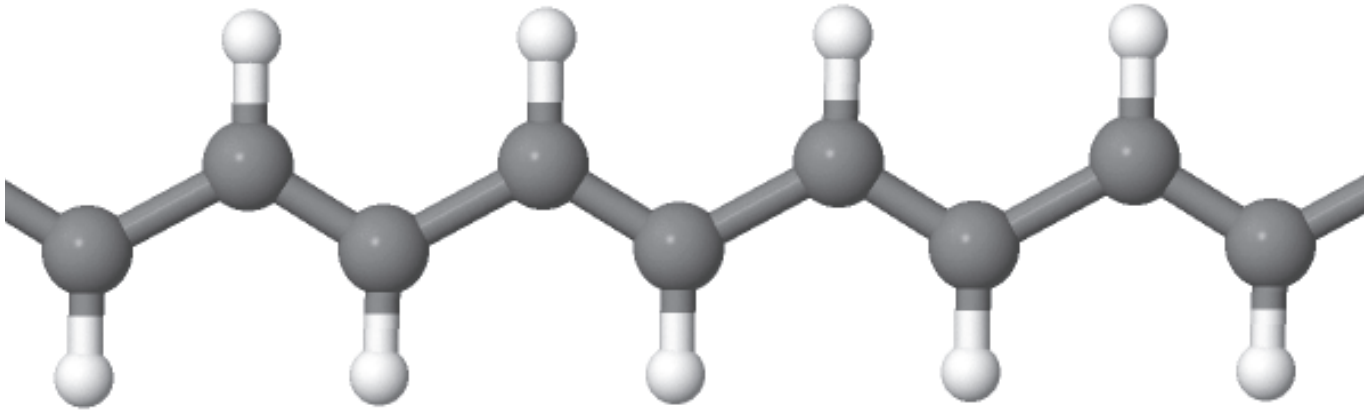
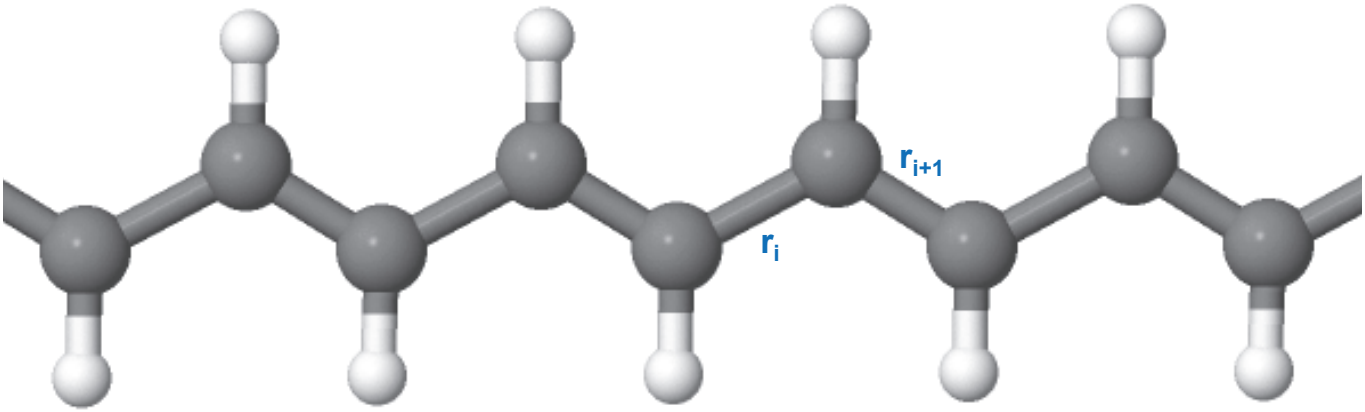
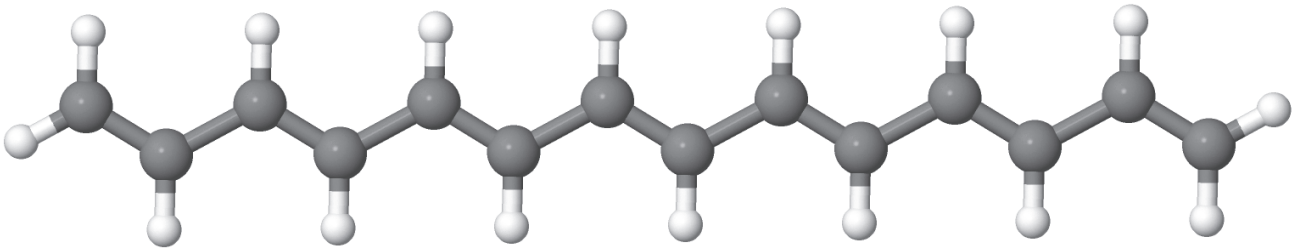


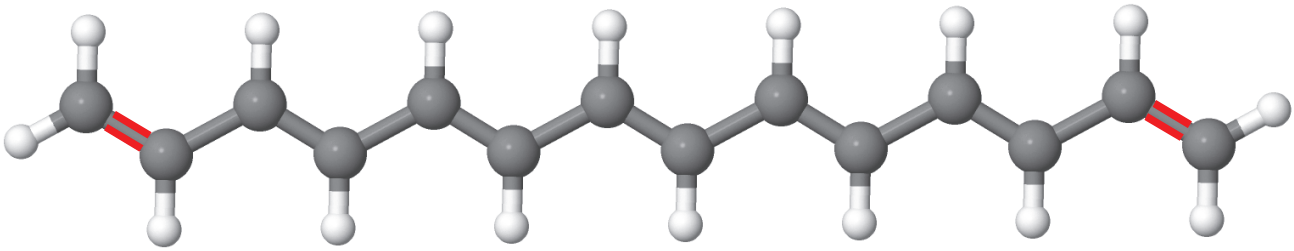
Bond Length Alternation: $BLA_i = |r_{i+1} - r_i|$



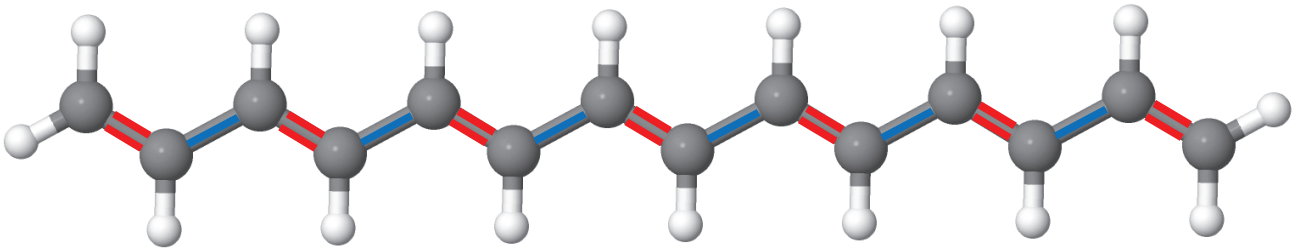
finite oligomer: chain end effects



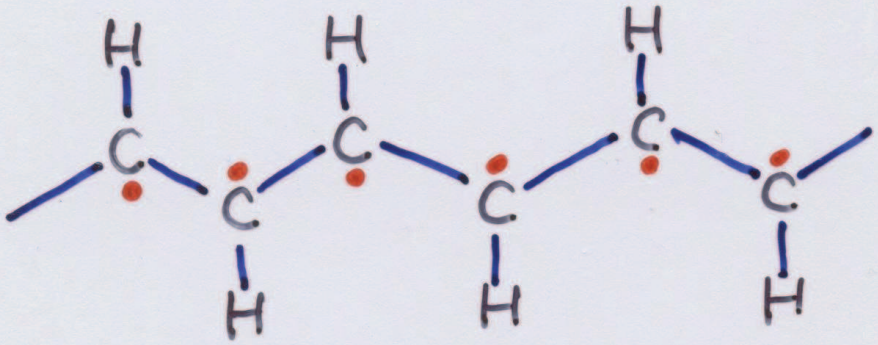
finite oligomer: chain end effects



finite oligomer: chain end effects



trans - POLYACETYLENE



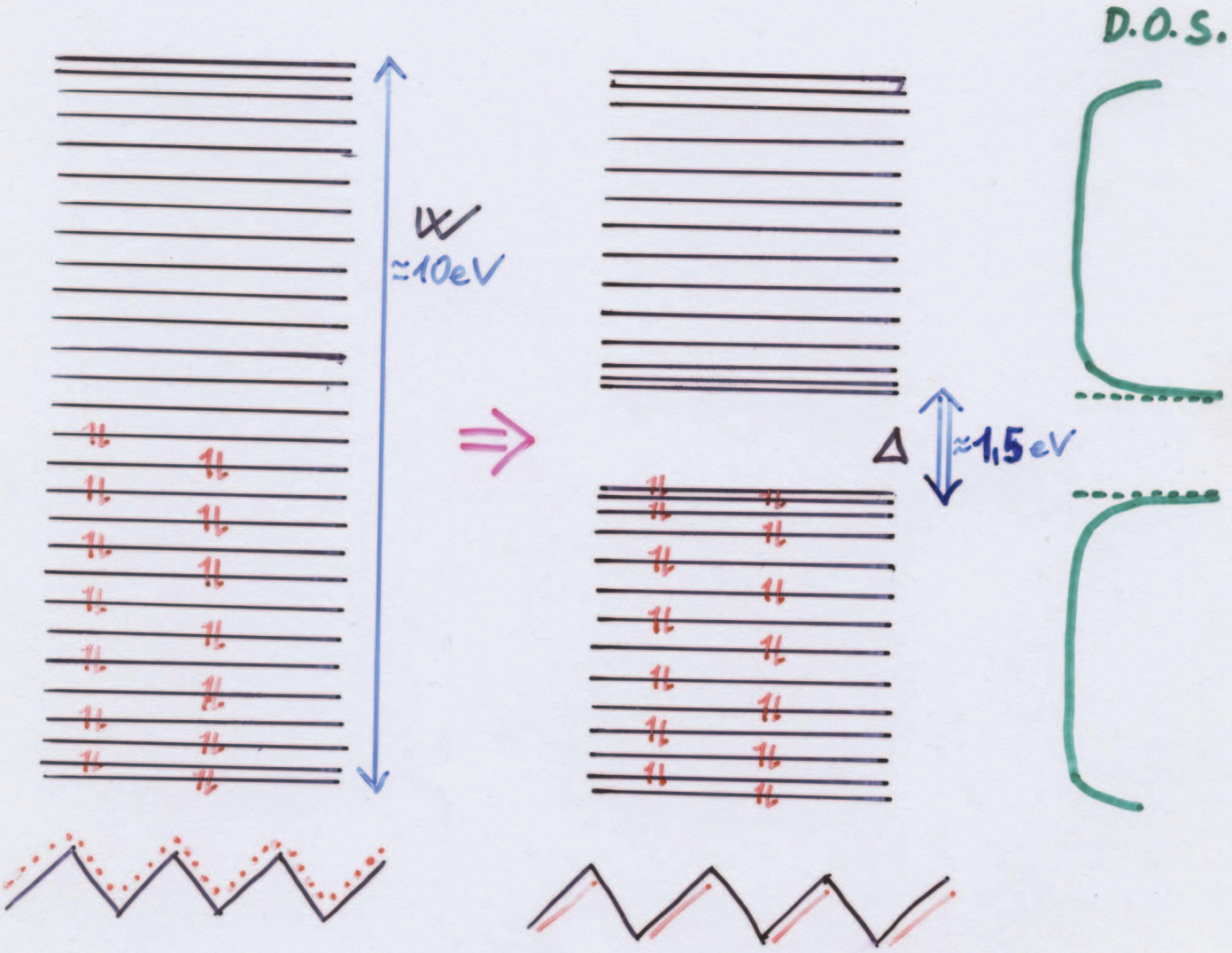
sp^2 hybrid orbital : 3 / carbon atom

→ σ - band, fully occupied

p_z orbital : 1 / carbon atom

→ π - band, half filled

trans - PA

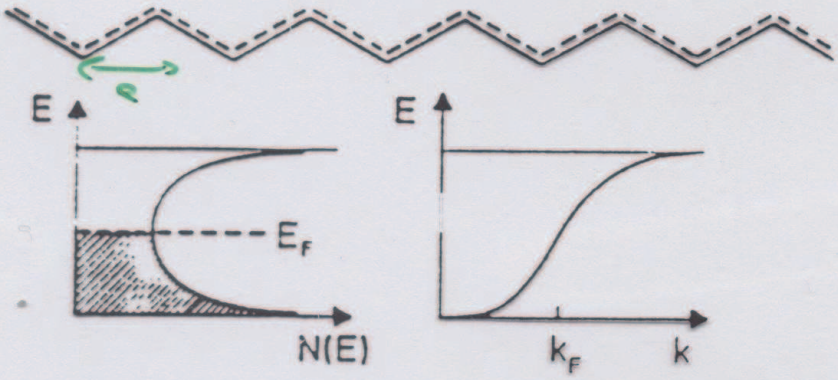


$r_{II} \approx 1{,}36\ \text{Å}$

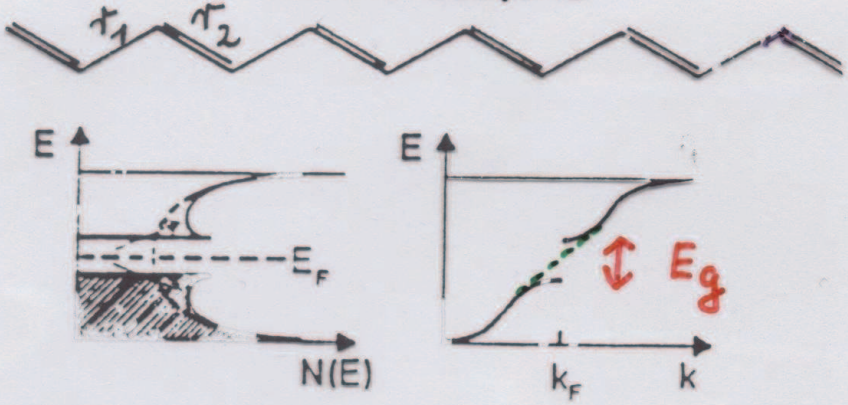
$r_{I} \approx 1{,}44\ \text{Å}$

Peierls instability in 1D

metallischer Zustand



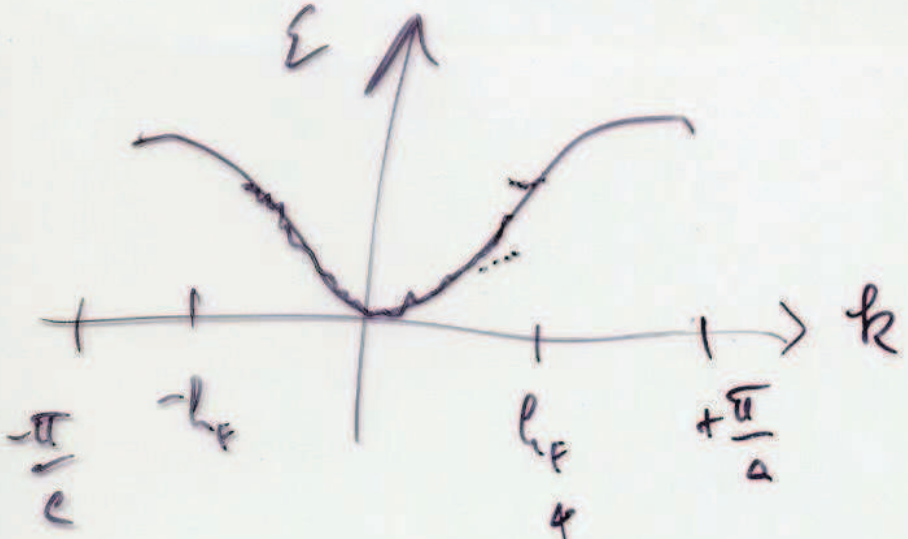
Isolatorzustand



$$\Delta r = r_1 - r_2$$

$$E_g \sim \Delta r$$

1dim instabilitások

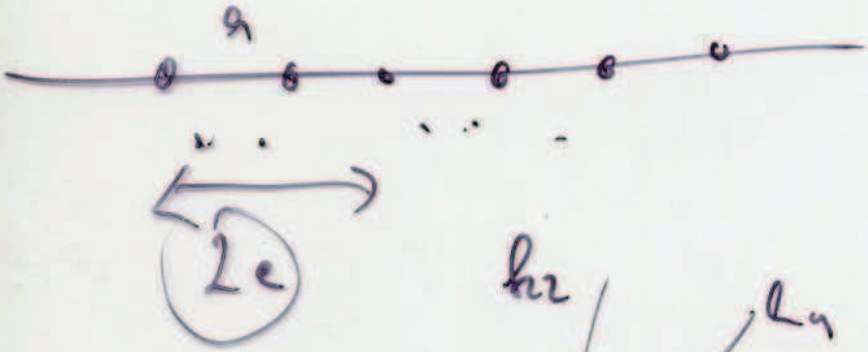


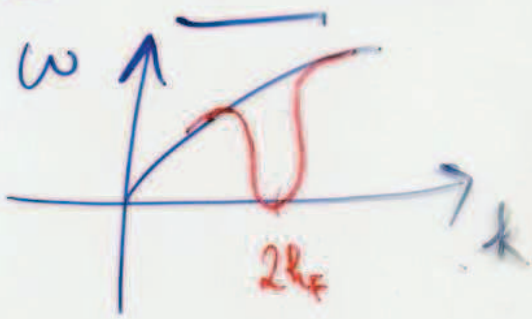
$2k_F$

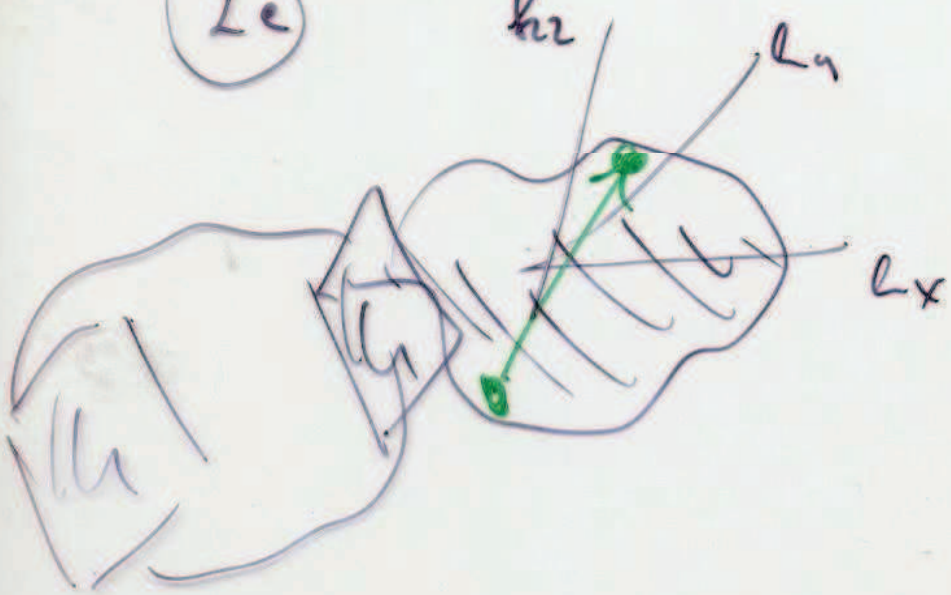
$\frac{\pi}{2a}$

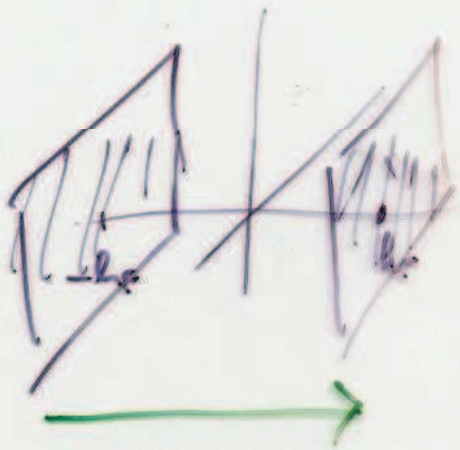
$2k_e = \frac{\pi}{a} = \frac{2\pi}{2a}$

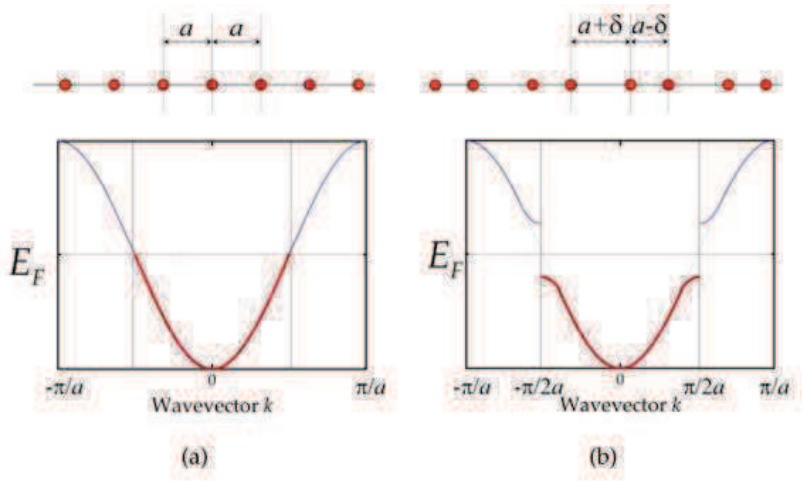
Peierls $\longleftrightarrow$ Kohn



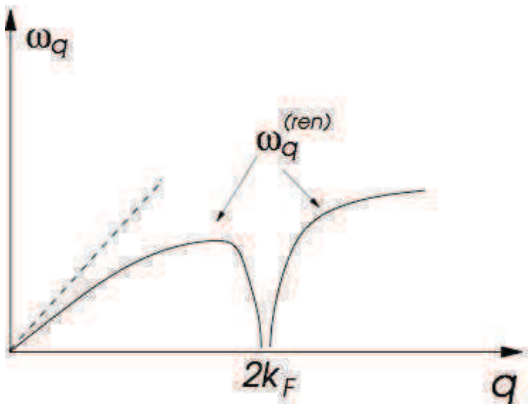






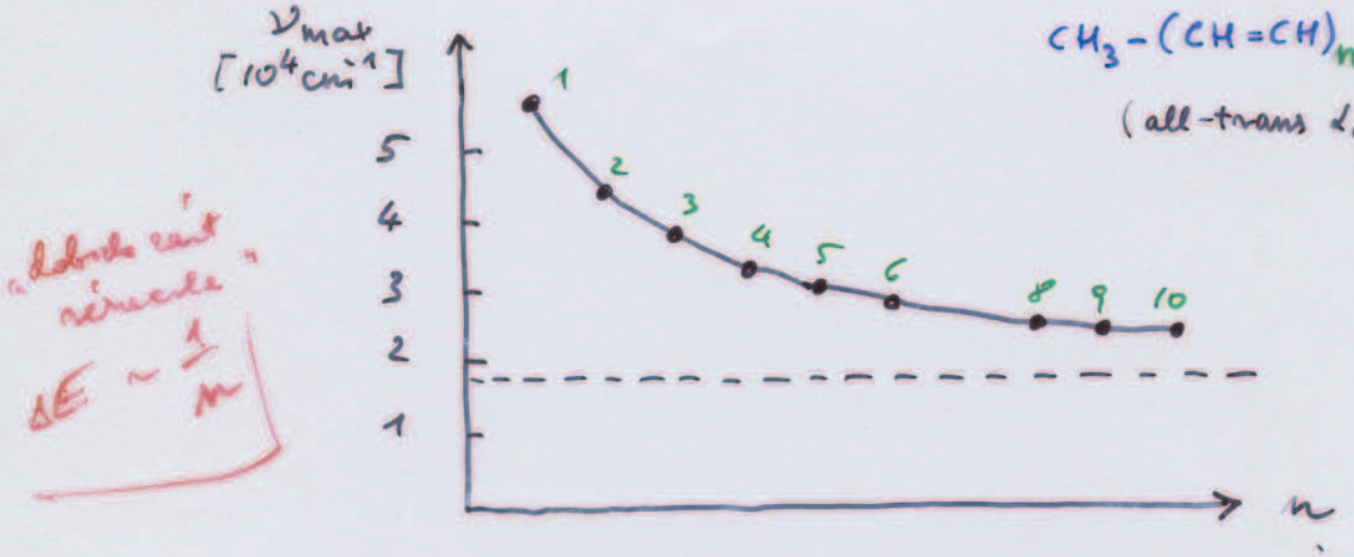


Peierls distortion (https://www.utwente.nl/tnw/pin/onderzoek/physical_properties_of_low-dimensional_systems/physical_properties_of_low-dimensional_systems-8.png)



Kohn anomaly (http://www.itp.phys.ethz.ch/education/fs14/sst/slides/Peierls.pdf)

i) gap



$CH_3-(CH=CH)_n-CH_3$

(all-trans α,ω dimethylpo

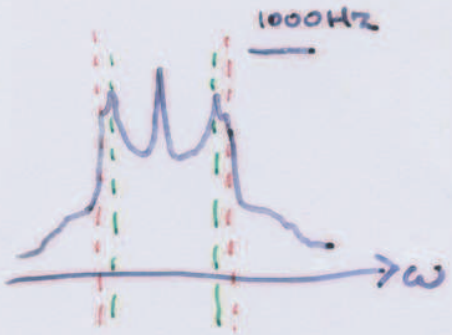
Konjugált polimerekben $E_g \approx 1{,}5-4$ eV

H_2C $=CH-CH$

ii) alternálás

$(CH)_x$ ^{13}C NMR (Yannoni, Clark)

Előállításnál: keverék $H-{}^{13}C\equiv{}^{13}C-H$ is!



Felhasadás dipól-dipól kh. miatt

$\Rightarrow$ $r_1 = 1{,}44$ Å

$r_2 = 1{,}36$ Å