

Peierls distortion

Distortion of a regular one-dimensional structure with a partially occupied band to give bond alternation, eventually leading to dimerization or oligomerization. The degree of oligomerization, λ depends on the electronic population of the conduction band indicated by the wave vector of the Fermi level k_F

$$\lambda = 2\pi/k_F$$

Note:

A Peierls distortion opens a gap at the Fermi level, producing a net stabilization of the distorted structure. The Peierls distortion for chain compounds is analogous to the Jahn–Teller effect for molecules. The prototypical example of the Peierls distortion in organic chemistry is the bond alternation present in polyvinylene.



Source:

PAC, 2007, 79, 293 (*Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006)*) on page 381