

Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Signatures of Dirac-Weyl fermions in long organic molecules¹

RICHARD KORYTAR, The Institute for Nanotechnology, Karlsruhe Institute of Technology, DIMITRA XENIOTI, Institut de Physique et de Chimie des Matériaux de Strasbourg (IPCMS), PETER SCHMITTECKERT², The Institute for Nanotechnology, Karlsruhe Institute of Technology, MEBAREK ALOUANI, Institut de Physique et de Chimie des Matériaux de Strasbourg (IPCMS), FERDINAND EVERS³, The Institute for Nanotechnology, Karlsruhe Institute of Technology — Oligoacenes are molecules which consist of N linearly fused benzene rings. They have been subject of intensive research since they were suspected to support correlated ground states with charge or spin ordering. In addition, they have been considered promising for technological application in organic electronics. We use ab-initio calculations in order to investigate how the optical gap of the molecule decreases with increasing length N . Intriguingly, we find that the limit of a metallic wire is reached with strong oscillations that exhibit periodicity with several periods that are not commensurate with the lattice symmetries. In particular, at certain magical values $N^*=10, 21, 32, \dots$ the gap is (almost) vanishing and revives again at intermediate values. An explanation will be offered in terms of a band-structure argument.

¹DFG-Center of Functional Nanostructures, DFG Priority Program 1243, HC3 - SCC cluster of the Karlsruhe Institute of Technology

²Second affiliation: DFG Center for Functional Nanostructures, Karlsruhe Institute of Technology (KIT)

³Second affiliation: Institut fuer Theorie der Kondensierten Materie, Karlsruhe Institute of Technology (KIT); Third affiliation: DFG-Center for Functional Nanostructures, Karlsruhe Institute of Technology (KIT)

Richard Korytar
The Institute for Nanotechnology, Karlsruhe Institute of Technology

Date submitted: 14 Nov 2013

Electronic form version 1.4