Universität Basel

Research Project

Open-Shell Graphene Fragment in a Shell: Stabilization of Fragile Triangulene Core

Third-party funded project

Project title Open-Shell Graphene Fragment in a Shell: Stabilization of Fragile Triangulene Core
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Department
Project start 01.09.2014
Probable end 31.10.2016
Status Completed

Graphene fragments made of exclusively carbon and hydrogen atoms are useful molecular models, which aid and abet our understanding of intrinsic phenomena occurring in graphene. The well-defined structure of these fragments allows us to investigate how the desired properties relate to the structure on a small scale first, before moving to extended two-dimensional carbon networks. Chemistry of graphene fragments is well documented in the literature, with the exception of one class of these *hydrocarbon* molecules, namely, the *"open-shell graphene fragments"*. Their unique triangular topology breaks the "alternating-double-bond rule" and, as a result, these molecules contain unpaired delocalized electrons. In general, an increase of the fragment size leads to a higher number of unpaired electrons. The main reason for which the open-shell graphene fragments have not been studied to a great extent is the extremely low stability of systems containing unpaired electrons, the so-called *free radicals*. The majority of reports on open-shell graphene fragments describe derivatives of the smallest fragment, monoradical phenalenyl (three fused benzene rings), and only a few examples mention its larger homolog, diradical triangulene (six fused benzene rings). In fact, only one derivative of triangulene composed of only carbon and hydrogen atoms has been described so far, however, it could only detected under strictly inert conditions and at low temperatures because of its instability. The objective of the proposed research is to synthesize and characterize a persistent derivative of triangulene and validate its triplet ground state in the solid state for the first time. The unpaired electrons in such open-shell systems can, in principle, serve as information carriers and potentially be used in the design of quantum information processing devices.

Keywords graphene fragment, open shell, triangulene
Financed by
University of Basel

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