Molecular Graphenoids with Pentagon-Heptagon Defects.

University of Stuttgart
Germany
Institute for Theoretical Chemistry

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Supervisor:
Robert Toews

Examiner:
Prof. Andreas Koehn

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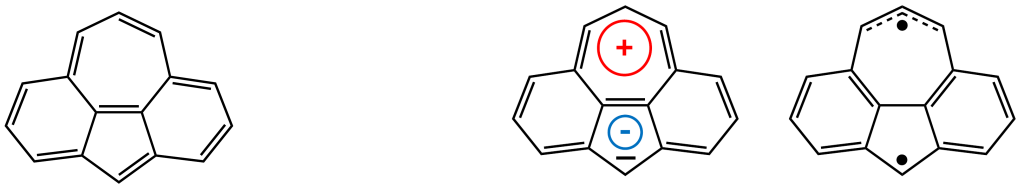
Motivation

Molecular graphenoids are planar, fully conjugated molecules that essentially resemble a fragment the hexagonal graphene lattice. The introduction of defects means a deviation of the actual molecular structure from the hexagonal carbon structure. In the case of pentagon-heptagon defects, two hexagons are formally replaced by a pentagon-heptagon pair. Cyclohepta[*def*]fluorene as shown in 1(a) can be considered as a simple example for a molecular graphenoid with pentagon-heptagon defect. In analogy to the familiar azulene molecule, the pentagon-heptagon defect establishes a substantial dipole moment in the closed-shell singlet state. Moreover, the closed-shell singlet state competes with an open-shell triplet state for the electronic ground state, *cf.* Figure 1(b).



(a) (b)

Figure 1: Chemical formula of cyclohepta[*def*]fluorene (a) and graphical representations (b) of closed-shell singlet and open-shell triplet state.

Regulation of electronic structure of molecules by external electric fields is a relevant topic in current research and bears significant potential for innovative technologies. Thereby, cyclohepate[*def*]fluorene can serve as simple reference system in order to obtain a basic mechanistic understanding of relevant effects.

Topic

This research project is focused on investigating the influence of external electric fields on the electronic structure of cyclohepta[*def*]fluorene and related molecular graphenoids. In particular, the effect on the equilibrium geometries of the electronic ground state and low-lying excited states is to be studied. For this purpose, density functional theory and multireference second-order perturbation theory are applied. Depending on the time schedule, additional aspects may be included such as excited state dynamics with an explicit consideration of relativistic effects.