Fullerene nanodiscs: from Chemistry to Combinatorics

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A graph is a mathematical model used to represent relationships between objects. The general characteristics that objects and their relationships can assume allowed the construction of the (so-called) Graph Theory, which has been applied to model large scale problems in several areas, such as Mathematics, Physics, Computer Science, Engineering, Chemistry and Psychology.

Fullerene graphs are mathematical models for carbon-based molecules experimentally discovered in the early 1980. Many parameters associated with these graphs have been discussed to describe the stability of fullerene molecules. By definition, fullerene graphs are cubic, planar, 3-connected with pentagonal and hexagonal faces. A total coloring of a graph assigns colors to the vertices and edges of a graph such that adjacent or incident elements have different colors. The famous Total Coloring Conjecture opened at 50 years, is settled for cubic graphs, but not to arbitrary regular graphs nor to arbitrary planar graphs. The length of the shortest cycle in a graph is called girth. Our goal is to study the total coloring of an infinite subfamily of fullerene graphs, the fullerene nanodiscs D_r, with distance between the inner (outer) layer and the central layer given by the radius parameter $r \geq 2$, motivated by a conjecture that the girth of a graph is a relevant parameter in the study of total coloring. To highlight the choice of the studied graph class, we present a historical scenario of the carbon molecule discovery that can be modeled through a special cubic planar graph of girth 5.

We provide a complete combinatorial description of the small fullerene nanodiscs. We prove that there is just one fullerene nanodisc with radius 2, just one fullerene nanodisc with radius 3, and just two fullerene nanodiscs with radius 4. We contribute by giving the first combinatorial description for fullerene nanodiscs, aiming to improve the understanding of this class, so that we are able to tackle the challenging total coloring of these graphs.

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