The conformable condition for Nanodiscs

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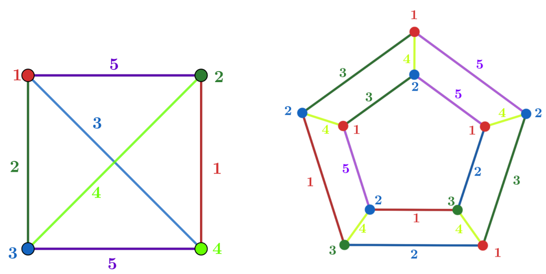
Abstract. *We investigate the total coloring of fullerene nanodiscs, a subclass of cubic planar graphs with girth* 5 *arising in Chemistry, motivated by a conjecture about the nonexistence of a Type 2 cubic graph of girth at least 5. We give a combinatorial description and then a conformable coloring for an infinite family of fullerene nanodiscs.*

1. The large girth Type 1 conjecture

A k-total coloring of a graph G is a color assignment from set $E \cup V$, where E denotes the set of edges and V denotes the set of vertices of the graph, such that distinct colors are assigned to: every pair of vertices that are adjacent; all edges that are adjacent; and each vertex and its incident edges. The total chromatic number $\chi''(G)$ is the smallest natural k for which G admits a k-total coloring. Behzad and Vizing [Behzad 1965, Vizing 1964] independently conjectured the Total Coloring Conjecture (TCC) that for any simple graph G, we have $\chi''(G) \leq \Delta(G) + 2$. If $\chi''(G) = \Delta(G) + 1$, then the graph is Type 1; if $\chi''(G) = \Delta(G) + 2$, then the graph is Type 2. The TCC has been verified for some particular classes of graphs, including cubic graphs [Kostochka 1996].



(a) (b)

Figure 1. (a) **A Type** 2 **girth 3 cubic graph;** (b) **a Type** 2 **girth 4 cubic graph.**

Every known Type 2 cubic graph has a girth 3 or 4 (See Figure 1). So, it is natural to think that there are no Type 2 cubic graphs with girth at least 5. Thus the following conjecture was proposed [Brinkmann et al. 2015]:

Conjecture 1. *There is no Type 2 cubic graph with girth at least 5.*

We will then define a special vertex coloring which is a necessary condition for a graph to be Type 1.

Lemma 1 ([Chetwynd and Hilton 1988])**.** *Let G be a regular graph. G is conformable if and only if it has a vertex coloring with $\Delta + 1$ colors and each color class has the same parity of $|V(G)|$.*

By Lemma 1, a necessary step towards proving that a cubic graph is Type 1 is to define a 4-vertex coloring where the cardinality of each vertex color class is even. Deciding whether an arbitrary graph is Type 1 is NP-complete [Sánchez-Arroyo 1989], even restricted to cubic graphs. Therefore, extending a conformable coloring to a $(\Delta + 1)$-total coloring is also NP-complete.

Lemma 2 ([Chetwynd and Hilton 1988])**.** *If G is a Type 1 graph, then G is conformable.*

2. The nanodiscs are graphs of girth 5

The fullerene nanodiscs, or nanodiscs D_r of radius $r \geq 2$, are structures composed of two identical flat covers, made with only hexagonal faces, connected by a strip along their borders constructed with additional 12 pentagonal faces. Figure 2 shows nanodiscs, where we highlighted with blue color in the connecting strip the 12 pentagonal faces.

The sequence $\{1, 6, 12, 18, ..., 6(r-1), 6r, 6(r-1), ..., 18, 12, 6, 1\}$ provides the amount of faces on each layer of the nanodisc graph D_r. The 12 pentagonal faces are distributed in the central layer among its $6r$ faces with the other $(6r - 12)$ hexagonal faces [Nicodemos 2017]. The auxiliary cycle sequence $\{C_6, C_{18}, \ldots, C_{12r-6}, C_{12r-6}, \ldots, C_{18}, C_6\}$ provides the sizes of the auxiliary cycles that define the layers. A nanodisc contains $12r^2$ vertices, $18r^2$ edges and has girth 5.

3. All even radius nanodiscs are conformable

A strategy to color the vertices of D_r is to take advantage that the auxiliary cycles have even length and color alternately with colors 1 and 2 the cycle C_6 defining the inner layer, with colors 3 and 4 the next cycle C_{18}, and so on. The strategy does not rely on the unicity of D_r, and defines for even radius a 4-vertex coloring that is conformable. See Figure 2.

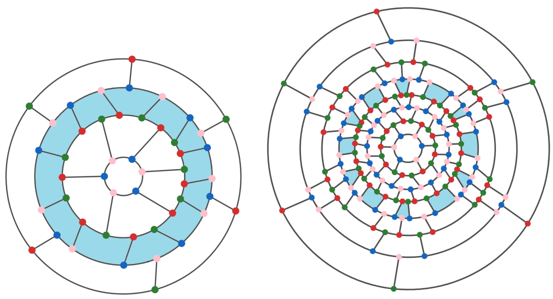


Figure 2. Conformable colorings for D_2 and D_4, respectively.

Theorem 1 ([da Cruz et al. 2021])**.** *Every nanodisc with even radius admits a conformable coloring.*

Proof. In a D_r with even r, consider the 4-vertex coloring that gives colors 1 and 2 to the outer cycle C_6, colors 3 and 4 to the next cycle C_{18}, until we reach the central layer, where colors 3 and 4 are given to cycle C_{12r-6} and colors 1 and 2 are given to the next cycle C_{12r-6}, continue in this fashion until colors 3 and 4 are given to the inner cycle C_6. There are $2r$ cycles, and each color appears in r cycles. Each color class has the same even number $3r^2$ of vertices. □

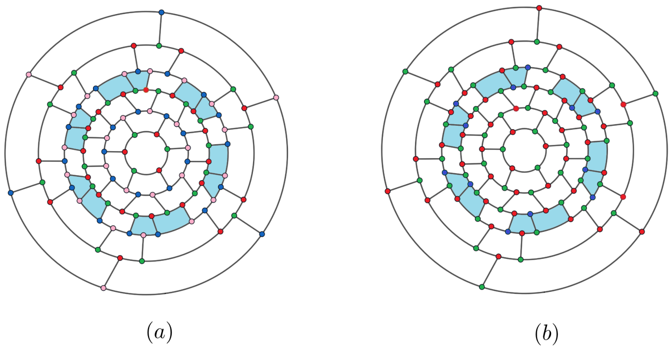


Figure 3. (a) A 4-vertex coloring that does not give a conformable coloring of D_3; (b) an optimal 3-vertex coloring that gives a conformable coloring of D_3.

Note that for r odd this 4-vertex coloring is not conformable, since $3r^2$ generates an odd number of vertices for each color class (See Figure $3(a)$). Thus, seeking to prove that all D_r nanodiscs are conformable, we further studied the D_3 nanodisc and obtained an optimal 3-vertex coloring that gives a conformable 4-vertex coloring, since each of the three color classes has an even number of vertices, and the fourth color class has 0 elements (See Figure $3(b)$).

Theorem 2 ([da Cruz et al. 2021])**.** *The nanodisc D_3 is conformable.*

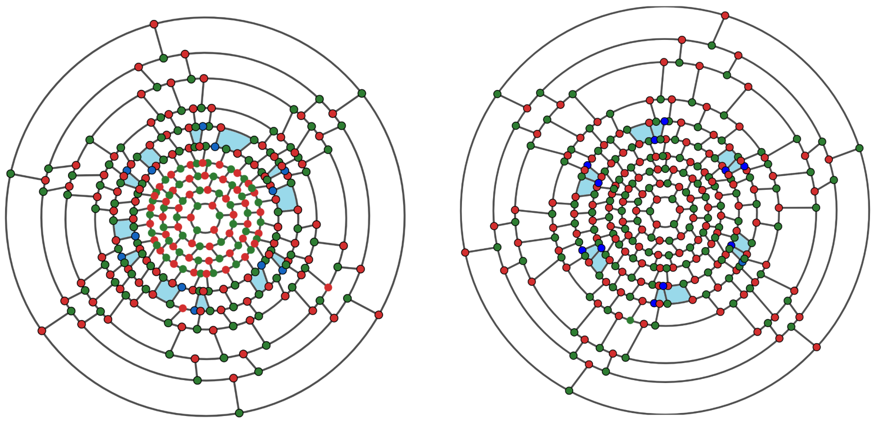


Figure 4. 3-vertex colorings of the two non-isomorphic instances of D_5.

The optimal 3-vertex coloring strategy for D_3 consists of coloring the auxiliary cycles, except for the two cycles of the center layer, using two colors alternately, avoiding color conflict in the vertices that are extremes of radial edges between consecutive auxiliary cycles. In the cycles C_{12r-6} defining the central layer, we introduce a third color by choosing six vertices in each cycle, thus ensuring the parity of this color class and the other color classes, where the fourth color class has 0 vertices. Recently, we have found two non-isomorphic instances for the fullerene nanodisc D_5. We verified the coloring strategy described above in both, which culminated in the following result (See Figure 4).

Theorem 3. *The two non-isomorphic instances of nanodisc D_5 are conformable.*

4. Current work

Our current goal is to generalize the 3-vertex coloring strategy that gives a conformable coloring of D_3 presented in Figure 3(b) and of D_5 presented in Figure 4 to an arbitrary nanodisc of odd radius. We were not able to extend the conformable vertex colorings defined in Section 3 for a 4-total coloring of those fullerene nanodiscs. We need to further investigate the structure of the class, looking for a suitable conformable vertex coloring that extends to a 4-total coloring of D_r, in order to prove that every fullerene nanodisc is Type 1, as has already been proven for D_2 [da Cruz et al. 2021]. See Figure 5.

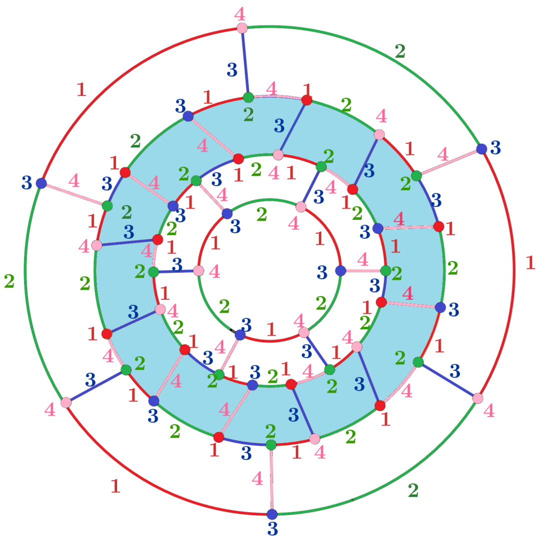


Figure 5. A 4-total coloring of D_2.

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