International Journal of Pure and Applied Mathematics
Volume 120 No. 8 2018, 207-215
ISSN: 1314-3395 (on-line version)
url: http://www.acadpubl.eu/hub/
Special Issue
http://www.acadpubl.eu/hub/

ADJACENT VERTEX DISTINGUISHING CHROMATIC INDEX OF CERTAIN NANO STRUCTURES

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Abstract

An adjacent vertex distinguishing edge coloring of a graph G is a proper edge coloring such that no two pair of adjacent vertices have the same set of colors, that is adjacent vertices are distinguished by their color set. The k-avd chromatic index of a graph G with maximum degree $\Delta(G)$, denoted by $\chi'_{avd}(G)$ is the minimum number k required in avd-edge coloring of G. This paper focuses on nanosheets whose $\chi'_{avd}(G)$ is equal to $\Delta(G)+1$ and $\Delta(G)+2$.

AMS Subject Classification: 05B40, 68R10.

Key Words and Phrases: AVD-chromatic index, chemical structures, $C_6[m,n]$, $C_4C_8(S)[2m,2n]$ nanosheets.

1 Introduction

Graph theory finds its applications in modelling chemical structures. A chemical (molecular) graph can be considered as a collection of vertices representing the atoms in the molecule and a set of edges representing the covalent bonds. Graph representation of molecular structures is widely used in computational chemistry [2, 8]. The edge colorings of graphs are shown to be useful in multiple quantum Nuclear Magnetic Resonance (NMR) from which one would obtain various types of dipolar couplings present in a molecule. The edge colorings of graphs are shown to enumerate unique dipolar interactions among a given set of nuclei there by providing a technique for structure elucidation from NMR [3, 8].

Let $G = (V, E)$ be a graph with vertex set V and edge set E. A proper edge coloring is a mapping $c : E \to N$ satisfying $c(xy) \neq c(yz)$ for any $xy, yz \in E$. For any $x \in V$, let $S(x)$ denote the set of colors of all edges incident to x. A proper edge coloring c is said to vertex distinguishing if $S(x) \neq S(y)$, for any $x, y \in V$ and $x \neq y$. Adjacent vertex distinguishing edge coloring is a relaxed version of vertex distinguishing in which only adjacent vertices are distinguished by their color set. Mathematically, an adjacent vertex distinguishing edge coloring is a proper edge coloring c satisfying $S(x) \neq S(y)$ for any x, y with $xy \in E$. The minimum number of colors k required for any AVD-edge coloring of G is called k-avd chromatic index of G and is denoted by $\chi'_{avd}(G)$ [6].

Vertex distinguishing proper edge coloring of graphs was first examined by Burris and Schelp [7] and further extended to adjacent vertex distinguishing edge coloring by Balister et al. [4, 5] Zhang et al. [12]. AVD-edge coloring is also studied in the name of adjacent strong edge coloring and 1-strong edge coloring [1]. In this paper, finite, simple and undirected graphs are considered and standard graph theoretic terminology is used.

2 Nanosheets with AVD-edge Coloring

Carbon nanosheets are a new kind of two dimensional polymeric material that is fabricated by cross linking aromatic self-assembled monolayers with electrons. Due to their uniform thickness of only about one nanometer, as well as their high chemical, mechanical and thermal stability, such materials are of high interest for a wide variety of applications. As the nanosheet is stable under an electron beam, patterns can also be written by electron beam induced deposition (EBID). The stability and flexibility nature of carbon nanosheet finds its multifold applications in sensors, filtration membranes, sample supports and even conductive coatings [9, 10, 11].

3 $C_6[m, n]$ Nanosheet

A $C_6[m, n]$ nanosheet is a trivalent decoration made by hexagons C_6 and is a biregular graph with m number of rows and n number of columns. It can also be redrawn in the form of bricks as shown in Fig. 1 and Fig. 2. A $C_6[m, n]$ nanosheet with wrap-around edges is called a $C_6[m, n]$ nanotube, also known as Peri-condensed Benzenoid Graph [10].

The $C_6[m, n]$ nanosheet has the vertex set $V = \{x_{ij}, 0 \leq i \leq m-1, 0 \leq j \leq n-1\}$ and the edge set $E = \{x_{2k-2,0}x_{2k-1,0}, x_{2k-2,2}x_{2k-1,2}, \ldots, x_{2k-2,2n}x_{2k-1,2n}\} \cup \{x_{2k-1,1}x_{2k,1}, x_{2k-1,3}x_{2k,3}, \ldots, x_{2k-1,2n-1}x_{2k,2n-1}\}$ with $1 \leq i \leq m$. The $C_6[m, n]$ nanosheet has $(4n + 2)m$ vertices, of which $4n$ are 2 degree vertices and $4n(m-1) + 2m$ are 3 degree vertices.

Let H_k be the sequence of horizontal edges defined by $H_k = \{x_{k1}, x_{k2}, \ldots, x_{kn}/1 \leq k \leq 2m\}$

Let V_k & V'_k be the sequence of vertical edges defined by

$$V_k = \{x_{2k-2,0}x_{2k-1,0}, x_{2k-2,2}x_{2k-1,2}, \ldots, x_{2k-2,2n}x_{2k-1,2n}\}$$
$$V'_k = \{x_{2k-1,1}x_{2k,1}, x_{2k-1,3}x_{2k,3}, \ldots, x_{2k-1,2n}x_{2k,2n-1}$$

with $1 \leq k \leq m$.

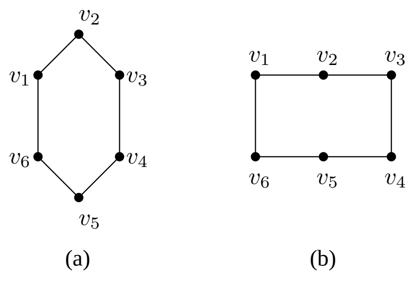

Figure 1: $C_6[1, 1]$ nanosheet (a) Hexagon form (b) Brick form

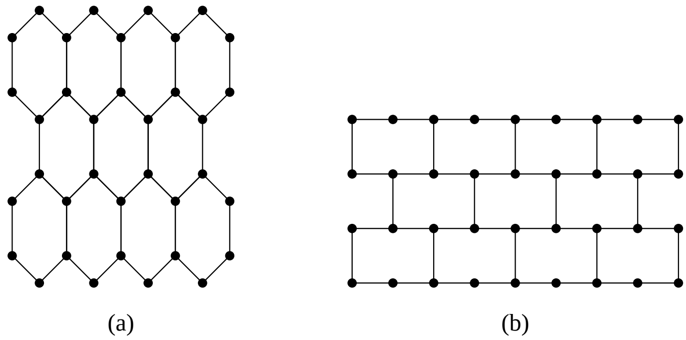

Figure 2: $C_6[3,4]$ nanosheet (a) Hexagon form (b) Brick form

Theorem 1. *Let G be a $C_6[m,n]$ nanosheet. Then* $\chi'_{avd}(G) = 4$.

Proof. We define the coloring c of horizontal edges as H_k, $1 \leq k \leq m$
$c(H_1) = (2,3,2,3,\dots)$
$c(H_i) = (c(H_{i-1}) + 1) \mod 4$ for $2 \leq i \leq 2n$
And the coloring of vertical edges V_k and V'_k as
$c(V_1) = (1,1,1,1,\dots)$
$c(V_j) = (c(V_{j-1}) + 2) \mod 4$ for $1 \leq i \leq m$
$c(V'_1) = (2,2,2,\dots)$
$c(V'_j) = (c(V_{j-1}) + 2) \mod 4$ for $1 \leq i \leq m-1$.
By construction c is a proper coloring. It remains to show c is an AVD-edge coloring.
Case 1: For any $x, y \in V$, if $deg(x) \neq deg(y)$ then $S(x) \neq S(y)$.
Case 2: For vertices of 2 degree. There are $4n$ vertices of degree 2. Since the initial (starting) and final (ending) edges of H_1 ae distinct, no two adjacent vertices of degree 2 have the same set of colors. Similarly, H_{2m} also has distinct color sets for adjacent 2 degree vertices.
Case 3: For vertices of 3 degree.

(i) $S(x_{i,j}) = (\alpha, \alpha+1, \beta)$ and $S(x_{i+1,j}) = (\alpha+1, \alpha+2, \beta)$ for some $\alpha, \beta \in \{0,1,2,3\}$ and addition is taken over modulo 4. Hence $S(x_{i,j}) \neq S(x_{i+1,j})$,

(ii) $S(x_{i,j}) = (\alpha, \alpha+1, \beta)$ and $S(x_{i,j+1}) = (\alpha, \alpha+1, \beta+1)$ for some

$\alpha, \beta \in \{0,1,2,3\}$ and addition taken on modulo 4. Hence $S(x_{i,j}) \neq S(x_{i,j+1})$

Therefore, for any adjacent vertices $x, y \in V[C_6[m,n]]$, $S(x) \neq S(y)$ as shown in Fig. 3. □

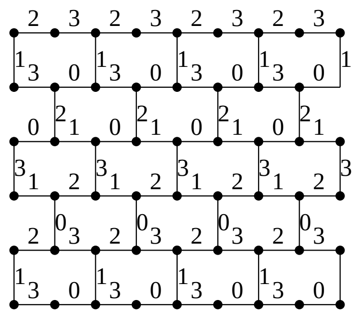

Figure 3: AVD-edge coloring of $C_6[3,4]$ nanosheet

4 $C_4C_8(S)[2m,2n]$ Nanosheet

A $C_4C_8(S)[2m,2n]$ nanosheet is a trivalent decoration made by alternating squares C_4 and octagon C_8 and a bi regular graph with m number of rows and n number of columns. It can also be redrawn in the form of bricks as shown in Fig. 4(a) and 4(b). It is a bipartite graph. The $C_4C_8(S)[2m,2n]$ nanosheet has $8mn$ vertices.

The vertex set of $C_4C_8(S)[2m,2n]$ is $V = \{x_{ij}/0 \leq i \leq m-1, 0 \leq j \leq n-1\}$ and the edge set $E = \{x_{2k-2,0}x_{2k-1,0}, x_{2k-2,3}x_{2k-1,3}, \ldots, x_{2k-2,4n-2}x_{2k-1,4n-1}\} \cup \{x_{2k-1,1}x_{2k,1}, x_{2k-1,2}x_{2k,2}, \ldots, x_{2k-1,4n-3}x_{2k-1,4n-2}\}$ with $1 \leq i \leq m$.

Theorem 2. *Let G be a $C_4C_8(S)[2m,2n]$ nanosheet. Then $\chi'_{avd}(G) = 5$.*

Proof. We define the coloring c of horizontal edges H_k as
$c(H_1) = (2,3,4,0,1,2,3,\ldots)$
$c(H_i) = (c(H_{i-1})+1) \mod 5$ for $2 \leq i \leq 2n$
and vertical edges V_k and V'_k, $1 \leq k \leq m$ as

$$V_k = \{x_{2k-2,0}x_{2k-1,0}, x_{2k-2,3}x_{2k-1,3}, \ldots, x_{2k-2,4n-2}x_{2k,4n-1})$$
$$V'_k = \{x_{2k-1,1}x_{2k,1}, x_{2k-1,2}x_{2k-1,2}, \ldots, x_{2k-1,4n-3}x_{2k-1,4n-2})$$

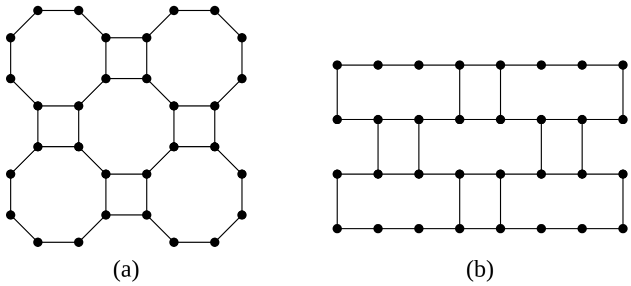

Figure 4: $C_4C_8(S)[2, 4]$ nanosheet (a) Octagon form (b) Brick form

By construction c is a proper coloring. It remains to show c is an AVD-edge coloring.
Case 1: For any $x, y \in V$, if $deg(x) \neq deg(y)$, then $S(x) \neq S(y)$.
Case 2: For vertices of degree 2. There are $4(m + n)$ vertices of degree 2. Since the starting and ending edges of H_1 are distinct, no two adjacent vertices of degree 2 have the same set of colors. Similarly, H_{2m} also has distinc color sets for adjacent 2 degree vertices.
Case 3: For vertices of degree 3.

(i) $S(x_{i,j}) = (\alpha, \alpha + 1, \beta)$ and $S(x_{i+1,j}) = (\alpha + 1, \alpha + 2, \beta)$ for some $\alpha, \beta \in \{0, 1, 2, 3, 4\}$ and addition taken over modulo 5. Hence $S(x_{i,j}) \neq S(x_{i+1,j})$

(ii) $S(x_{i,j}) = (\alpha, \alpha + 1, \beta)$ and $S(x_{i,j+1}) = (\alpha + 1, \alpha + 2, \beta + 2)$ modulo 5. Hence $S(x_{i,j}) \neq S(x_{i,j+1})$

Therefore, for any adjacent vertices $x, y \in V[C_4C_8(S)[2m, 2n]]$, $S(x) \neq S(y)$ as shown in Fig. 5. □

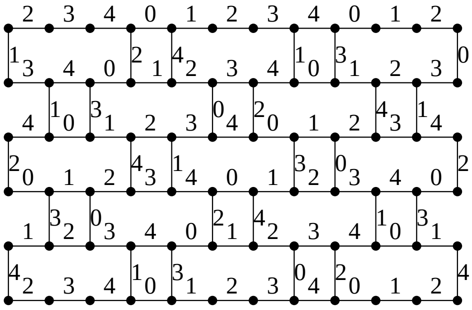

Figure 5: AVD-edge coloring of $C_4C_8(S)[6,6]$ nanosheet

5 Conclusion

In this paper, we have proved that avd-chromatic index of $C_6[m,n]$ nanosheet is $\Delta(G)+1$ and $C_4C_8(S)[m,n]$ nanosheet is $\Delta(G)+2$. The AVD-edge coloring of other nanosheets are under investigation.

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