Research Article

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An estimation of HOMO–LUMO gap for a class of molecular graphs

https://doi.org/10.1515/mgmc-2022-0011
received March 11, 2022; accepted May 31, 2022

Abstract: For any simple connected graph G of order n, having eigen spectrum $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$ with middle eigenvalues μ_H and μ_L, where $H = \lfloor (n+1)/2 \rfloor$ and $L = \lceil (n+1)/2 \rceil$, the HOMO–LUMO gap is defined as as $\Delta G = \mu_H = \mu_L$. In this article, a simple upper bound for the HOMO–LUMO gap corresponding to a special class of connected bipartite graphs is estimated. As an application, the upper bounds for the HOMO–LUMO gap of certain classes of nanotubes and nanotori are estimated.

Keywords: molecular graph, eigen spectrum, HOMO–LUMO gap, bipartite graphs, Hermitian matrix

1 Introduction

Let G be a simple connected graph on n vertices. The eigenvalues of G, $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$ are the eigenvalues of adjacency matrix $A(G)$ of graph G arranged in descending order as $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$ and is referred to as eigen spectrum of G. The eigen spectrum of different families of graphs is widely studied. There is extensive work on finding the smallest, largest, and middle eigenvalues of the graph in literature. The middle eigenvalues have a great deal in theoretical chemistry, especially in the Huckel molecular orbital model of Π-electron system. For graph G, let $H = \lfloor (n+1)/2 \rfloor$ and $L = \lceil (n+1)/2 \rceil$. Then, HOMO–LUMO gap is defined as $\Delta_G = \mu_H - \mu_L$. HOMO and LUMO denote highest occupied molecular orbital and lowest unoccupied molecular orbital, respectively. HOMO–LUMO gap relates to the kinetic stability of molecules. The larger the value of HOMO–LUMO, the higher the kinetic stability and the lower the chemical reactivity. As a number of molecular graphs, like acyclic alkanes, certain nanotubes and so on, are bipartite so it is important to study the HOMO–LUMO gap on bipartite graphs in general.

Any bipartite graph G with its vertex set $V(G)$ can be partitioned into two classes of starred and un starred vertices that is $V^*(G) = \{v_1, v_2, \cdots, v_r\}$ and $V(G) = V^o(G) = \{v_{r+1}, v_{r+1}, \cdots, v_n\}$, respectively. The bi adjacency matrix of G is the $r \times (n-r)$ matrix $B(G) = (b_{ij})$, where $b_{ij} = 1$, if $v_i v_j \in E(G)$, $v_i \in V^*(G)$ and $v_j \in V^*(G)$ and otherwise $b_{ij} = 0$. The adjacency matrix of the graph G can be written as:

$$A(G) = \begin{pmatrix} O & B \\ B^T & O \end{pmatrix}$$

Mohar (2013) proved that the median eigenvalues of every bipartite planar graph of maximum degree at most three belong to the interval $[-1, 1]$, and Mohar (2016) showed that the same result holds for all bipartite graphs of degree at most three except Heawood graph whose median eigenvalues are $\pm\sqrt{2}$. Later, Mohar (2015) provided rather tight lower and upper bounds on the maximum value of the HOMO–LUMO index among all graphs with a given average degree. In the study by Mohar and Tayfeh-Rezaie (2015), the upper bound of maximum median eigenvalues (HOMO–LUMO index) of connected bipartite graphs with maximum degree $\Delta(G) \geq 3$ is estimated. Jaklic et al. (2012) studied bounds on HOMO–LUMO index for chemical and general graphs and exhibited the existence of graphs with sufficiently large HOMO–LUMO index. For more details on the HOMO–LUMO index and HOMO–LUMO maps, refer to Fowler and Pisanksi (2010a, 2010b) and Li et al. (2013). So far, not much work has been done on the HOMO–LUMO gap. The bounds for the HOMO–LUMO gap for sub-graphenic and sub-buckytubic species are estimated by Klein et al. (2015). In Ahmad and Hameed (2018), the bounds for C_4C_8 nanotubes and nanotoros are proposed. The polyenes with maximum HOMO–LUMO gap were studied in Fowler et al. (2001). HOMO–LUMO gaps

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and molecular structures of polycyclic aromatic hydrocarbons in soot formation were discussed by Xu et al. (2021). The aim of this article is to find the upper bound of HOMO–LUMO gap for a specific class of connected bipartite graphs.

Let B be the set of connected bipartite graphs. For any graph G belonging to B whose vertices are partitioned into $V^{**}(G)$ and $V^{\circ}(G)$, we construct two new graphs $G^{\star}$ and $G^{\circ\circ}$ by drawing an edge corresponding to each path of length 2 between any two vertices of $V^{**}(G)$ (respectively $V^{\circ}(G)$). For example, consider a tree on 14 vertices which is connected bipartite graph which is shown in Figure 1. The corresponding graphs $T_{14}^{\star}$ and T_{14}° are shown in Figures 2 and 3, respectively.

Let $\mathcal{H}$ denote the class of connected bipartite graph G for which the corresponding graphs $G^{\star}$ (respectively G°) is four partite, i.e.

$$\mathcal{H} = \{G \in B : G^{\star}(\text{respectively } G^{\circ} \text{ is four partite})\}$$

Since the graphs $T_{14}^{\star}$ and T_{14}° shown in Figures 2 and 3 are four partite, the graph T_{14} as shown in Figure 1 belongs to class $\mathcal{H}$. For $G \in \mathcal{H}$, V^{**} can be partitioned into four classes $V_{\alpha}^{\star}$, $V_{\beta}^{\star}$, $V_{\gamma}^{\star}$, and $V_{\delta}^{\star}$ in which the vertices of one class are adjacent to the vertices of remaining three classes only, and similarly, the vertex set V° can be partitioned into four classes.

In Section 2, the upper bounds of the HOMO–LUMO gap for the class $\mathcal{H}$ are estimated, and as an application in Section 3, the upper bounds for the HOMO–LUMO gap for the special class of nanotubes and nanotori $C_4(m,n)$ and $\mathrm{HRC}_4(S)(m,n)$, where $m, n > 1$ are estimated.

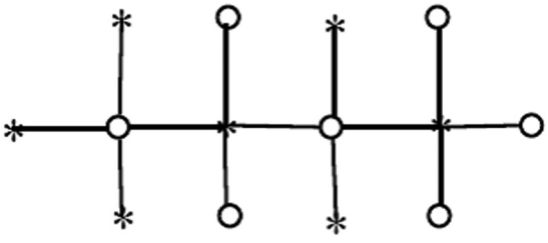

Figure 1: Tree T_{14}.

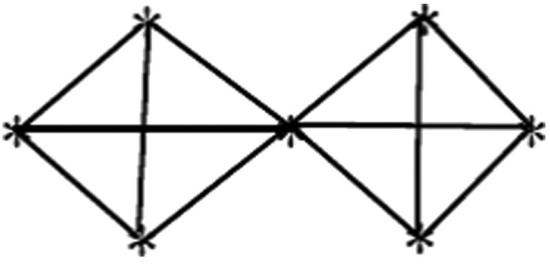

Figure 2: Graph $T_{14}^{\star}$.

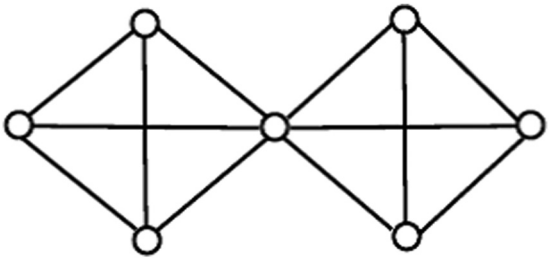

Figure 3: The graph T_{14}°.

Theorem 1.1. (Rayleigh Ritz quotient)
Let $M \in C^{n\times n}$ be a Hermitian matrix. Then, the least eigenvalue $\mu_{\min}(M)$ of M is:

$$\mu_{\min}(M) = \min_{v\in C^n,\, v\neq 0} \frac{v^{\dagger}Mv}{v^{\dagger}v}$$

where $v^{\dagger}$ denotes the conjugate transpose of v. Further, we often abbreviate $V(G)$, $E(G)$, $V^{\star}(G)$, $V^{\circ}(G)$, $A(G)$, and $B(G)$ to V, E, $V^{\star}$, V°, A and B, respectively.

2 Upper bound for the HOMO–LUMO gap of the class $\mathcal{H}$

For any $G \in \mathcal{H}$, the graph $G^{\star}$ is four partite in which the vertices in one class are adjacent to the remaining three classes only, and the adjacency matrix of $G^{\star}$ is given in Lemma 2.1.

Lemma 2.1. *For any $G \in \mathcal{H}$, the adjacency matrix of $G^{\star}$ is given by:*

$$A(G^{\star}) = \begin{pmatrix} O & A_{\alpha\beta} & A_{\alpha\gamma} & A_{\alpha\delta} \\ A_{\alpha\beta}^{T} & O & A_{\beta\gamma} & A_{\beta\delta} \\ A_{\alpha\gamma^{T}} & A_{\beta\gamma}^{T} & O & A_{\gamma\delta} \\ A_{\alpha\delta^{T}} & A_{\beta\delta}^{T} & A_{\gamma\delta}^{T} & O \end{pmatrix}$$

where each entry $A_{\omega\eta} = (d_{ij})$ of $A(G^{\star})$ is a matrix defined as d_{ij} = the number of edges between $V_i \in V_{\omega}^{\star}$ and $V_j \in V_{\eta}^{\star}$ in $G^{\star}$. As the adjacency matrix $A(G)$ of $G \in B$ can be written as:

$$A(G) = \begin{pmatrix} O & B \\ B^{\mathrm{T}} & O \end{pmatrix}$$

Therefore, the eigenvalues of A^2 are the eigenvalues of $C^{\star}$ and C° where $C^{\star} = BB^{T}$ and $C^{\circ} = B^{T}B$.

Lemma 2.2. *The matrix $C^\star$ corresponding to the graph $G \in \mathcal{H}$ is given by:*

$$C^\star = \begin{pmatrix} D_\alpha & A_{\alpha\beta} & A_{\alpha\gamma} & A_{\alpha\delta} \\ A_{\alpha\beta}^T & D_\beta & A_{\beta\gamma} & A_{\beta\delta} \\ A_{\alpha\gamma}^T & A_{\beta\gamma}^T & D_\gamma & A_{\gamma\delta} \\ A_{\alpha\delta}^T & A_{\beta\delta}^T & A_{\gamma\delta}^T & D_\delta \end{pmatrix}$$

where D_α, D_β, D_γ, and D_δ are diagonal matrices with diagonal entries as vertex degrees, and each entry $A_{\omega\eta} = (d_{ij})$ of $C^\star$ is a matrix where d_{ij} is the number of edges between $V_i \in V_\omega^\star$ and $V_j \in V_\eta^\star$ and in $G^\star$.

Lemma 2.3. *Let $G \in B$ be a connected bipartite graph, $\mu_{\min}(C^\star)$ and $\mu_{\min}(C^\circ)$ be the least eigenvalues of $C^\star$ and C°, respectively. Then:*

$$\Delta(G) = 2\min\{\sqrt{\mu_{\min}(C^\star)},\ \sqrt{\mu_{\min}(C^\circ)}\}$$

where $C^\star$ and C° are defined as above.

Theorem 2.1. *For the matrix $C^\star$ of the graph $G \in \mathcal{H}$, the minimum eigenvalue of $C^\star$ satisfies:*

$$\mu_{\min}(C^\star) \le \frac{|E(G)| - |E(G^\star)|/3}{|V^\star|}$$

Proof. Let $V_J^\star$, where $J \in \{\alpha, \beta, \gamma, \delta\}$ has j elements, and let V_j be the column vectors of order $j \times 1$ all of whose entries are 1 s. Further, suppose $M_{ij}^\star$ denotes the number of edges between $V_I^\star$ and $V_J^\star$, where $I, J \in \{\alpha, \beta, \gamma, \delta\}$ and:

$$M_{\gamma\delta}^\star = \max_{I,J\in\{\alpha,,\beta,\gamma,\delta\}}(M_{IJ}^\star)$$

Consider the fourth roots of unity, i.e., $\{1, -1, \epsilon, \epsilon^2\}$ with ϵ and ϵ^2 conjugate to each other and:

$$V = \begin{pmatrix} \epsilon V_\alpha \\ \epsilon^2 V_\beta \\ V_\gamma \\ -V_\delta \end{pmatrix}.$$

Then we have:

$$V^\dagger V = (\epsilon^2 V_\alpha^T \ \in V_\beta^T\ V_\gamma^T\ -V_\delta^T)\begin{pmatrix} \epsilon V_\alpha \\ \epsilon^2 V_\beta \\ V_\gamma \\ -V_\delta \end{pmatrix}$$

$$\begin{aligned} V^\dagger V &= V_\alpha^T V_\alpha + V_\beta^T V_\beta + V_\gamma^T V_\gamma + V_\delta^T V_\delta \\ &= |\alpha| + |\beta| + |\gamma| + |\delta| = |V^\star| \end{aligned}$$

$$V^\dagger C^\star V = (\ \epsilon^2 V_\alpha^T\ \epsilon V_\beta^T\ V_\gamma^T\ -V_\delta^T)\begin{pmatrix} D_\alpha & A_{\alpha\beta} & A_{\alpha\gamma} & A_{\alpha\delta} \\ A_{\alpha\beta}^T & D_\beta & A_{\beta\gamma} & A_{\beta\delta} \\ A_{\alpha\gamma}^T & A_{\beta\gamma}^T & D_\gamma & A_{\gamma\delta} \\ A_{\alpha\delta}^T & A_{\beta\delta}^T & A_{\gamma\delta}^T & D_\delta \end{pmatrix}\begin{pmatrix} \epsilon V_\alpha \\ \epsilon^2 V_\beta \\ V_\gamma \\ -V_\delta \end{pmatrix}$$

$$\begin{aligned} V^\dagger C^\star V = (&V_\alpha^T D_\alpha V_\alpha + \epsilon V_\alpha^T A_{\alpha\beta} V_\beta + \epsilon^2 V_\alpha^T A_{\alpha\gamma} V_\gamma - \epsilon^2 V_\alpha^T A_{\alpha\delta} V_\delta) \\ &+ (\epsilon^2 V_\beta^T A_{\alpha\beta}^T V_\alpha + V_\beta^T D_\beta V_\beta + \epsilon V_\beta^T A_{\beta\gamma} V_\gamma - \epsilon V_\beta^T A_{\beta\delta} V_\delta) \\ &+ (\epsilon V_\gamma^T A_{\alpha\gamma}^T V_\alpha + \epsilon^2 V_\gamma^T A_{\beta\gamma}^T V_\beta + V_\gamma^T D_\gamma V_\gamma - V_\gamma^T A_{\gamma\delta} V_\delta) \\ &- (\epsilon V_\delta^T A_{\alpha\delta}^T V_\alpha + \epsilon^2 V_\delta^T A_{\beta\delta}^T V_\beta + V_\delta^T A_{\gamma\delta} V_\gamma - V_\delta^T D_\delta V_\delta) \end{aligned}$$

$$\begin{aligned} V^\dagger C^\star V = (&V_\alpha^T D_\alpha V_\alpha + V_\beta^T D_\beta V_\beta + V_\gamma^T D_\gamma V_\gamma + V_\delta^T D_\delta V_\delta) \\ &+ (\epsilon V_\alpha^T A_{\alpha\beta} V_\beta + \epsilon^2 V_\beta^T A_{\alpha\beta}^T V_\alpha) \\ &+ (\epsilon^2 V_\alpha^T A_{\alpha\gamma} V_\gamma + \epsilon V_\gamma^T A_{\alpha\gamma}^T V_\alpha) \\ &- (\epsilon^2 V_\alpha^T A_{\alpha\delta} V_\delta + \epsilon V_\delta^T A_{\alpha\delta}^T V_\alpha) \\ &+ (\epsilon V_\beta^T A_{\beta\gamma} V_\gamma + \epsilon^2 V_\gamma^T A_{\beta\gamma}^T V_\beta) \\ &- (\epsilon V_\beta^T A_{\beta\delta} V_\delta + \epsilon^2 V_\delta^T A_{\beta\delta}^T V_\beta) \\ &- (V_\gamma^T A_{\gamma\delta} V_\delta + V_\delta^T A_{\gamma\delta} V_\gamma) \end{aligned}$$

$$\begin{aligned} V^\dagger C^\star V = &\left(\sum_{v_i} \epsilon V_\alpha^\star d_{v_i}(G)\right) + \left(\sum_{v_i} \epsilon V_\beta^\star d_{v_i}(G)\right) \\ &+ \left(\sum_{v_i} \epsilon V_\gamma^\star d_{v_i}(G)\right) + \left(\sum_{v_i} \epsilon V_\delta^\star d_{v_i}(G)\right) \\ &+ (\epsilon M_{\alpha\beta}^\star + \epsilon^2 M_{\alpha\beta}^\star) + (\epsilon^2 M_{\alpha\gamma}^\star + \epsilon M_{\alpha\gamma}^\star) \\ &- (\epsilon^2 M_{\alpha\delta}^\star + \epsilon M_{\alpha\delta}^\star) + (\epsilon M_{\beta\gamma}^\star + \epsilon^2 M_{\beta\gamma}^\star) \\ &- (\epsilon M_{\beta\delta}^\star + \epsilon^2 M_{\beta\delta}^\star) - (M_{\gamma\delta}^\star + M_{\gamma\delta}^\star) \end{aligned}$$

Hence, we can write:

$$V^\dagger C^\star V = \sum_{v_i} \epsilon V^\star d_{v_i}(G) - 2M_{\gamma\delta}^\star \le (|E(G)| - |E(G^\star)|/3)$$

Using Theorem 1.2 (Rayleigh Ritz quotient):

$$\mu_{\min}(M) = \mu_{\min}(M) = \min_{v\in C^n,\, v\neq 0} \frac{v^\dagger M v}{v^\dagger v} \le \frac{|E(G)| - \frac{|E(G^\star)|}{3}}{|V^\star|}$$

Now, using Lemma 2.3 and Theorem 2.1, we have Corollary 2.1.

Corollary 2.1. *For any graph $G \in \mathcal{H}$:*

$$\Delta(G) \le 2\min\{\sqrt{|E(G)| - |E(G^\star)|/3)/|V^\star|},\ \sqrt{|E(G)| - |E(G^\circ)|/3)/|V^\circ|}\}$$

3 Applications

Iijima (1991) discovered carbon nanotubes (CNTs) as multi-walled structures. These nanostructures are allotropes of carbon in a cylindrical shape. CNTs exhibit remarkable mechanical characteristics and are found to be one of the stiffest and most elastic known materials. Nanotubes are studied extensively in solid-state physics due to their immense applications in nanotechnology, electronics, optics, materials science, and architecture. In this section, the upper bounds for HOMO–LUMO gap of two families of nanotubes and nanotori, one is covered by C_4 (squares) and other is covered by rhombus; i.e., $C_4[m,n]$ and $HRC_4[m,n]$ are estimated. The two-dimensional (2D)-lattice of first family of nanotubes and nanotori is a plane arrangement of C_4 (square). The tilling of C_4 can cover either a cylinder (nanotube) or a torus (nanotorus). This family of nanotubes is denoted by $TUC_4[m,n]$, in which m is the number of squares in a row and n is the number of squares in a column. A 2D representation of $TUC_4[m,n]$ nanotube is depicted in Figure 4. Let G be the molecular graph of a C_4 (square) lattice. The graph is bipartite, and its vertex set $V(G)$ can be partitioned into two classes $V^{\star}(G)$ and $V^{\circ}(G)$ consisting of starred and circled vertices. Now, we construct starred graph $G^{\star}$ (respectively circled G°) by drawing an edge corresponding to each path of length 2 between any two starred (respectively circled) vertices of G. The graph $G^{\star}$ is in fact C_3C_4 net and is four partite. It is shown in Figure 5. Hence, the vertex set $V^{\star}(G)$ partitions into four classes $V_{\alpha}^{\star}$, $V_{\beta}^{\star}$, $V_{\gamma}^{\star}$, and $V_{\delta}^{\star}$ in

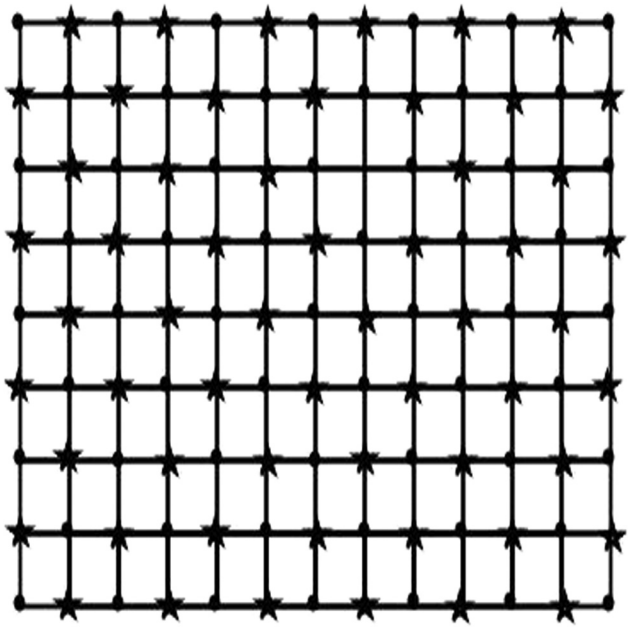

Figure 4: 2D representation of $TUC_4[12,8]$ nanotube.

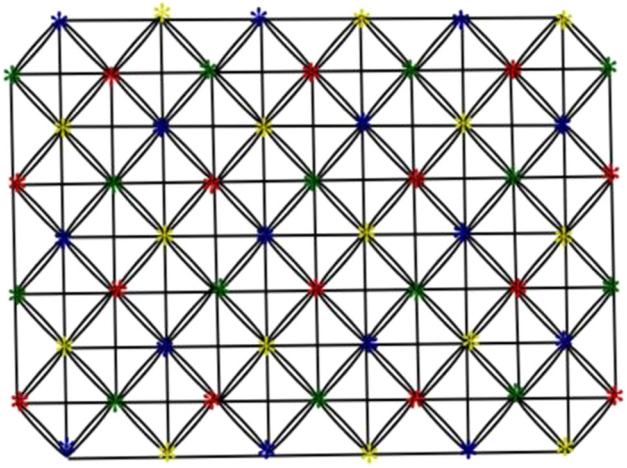

Figure 5: Starred graph G^{*} of $TUC_4[12,8]$ nanotube.

which the vertices of one class are adjacent to the vertices of the remaining three classes only, and similarly, the vertex set $V^{\circ}(G)$ can be partitioned into four classes.

Theorem 3.1. *For $m \cdot n \in N - \{1\}$ and $m,\ n \equiv 0(mod\ 4)$, let N and H be molecular graphs of nanotube $TUC_4[m, n]$ and nanotorus $C_4[m, n]$. Then:*

$$\Delta(N) \leq 2\sqrt{2}$$

and

$$\Delta(\mathrm{H}) \leq 2\sqrt{2}$$

Proof. The edge set cardinalities of N, $N^{\star}$, H, $H^{\star}$, and vertex set cardinalities of $N^{\star}$, $H^{\star}$ are given as follows:

$$|E(N)| = 2mn + m$$

$$|E(N^{\star})| = 2mn + \frac{m(n+1)}{2} + \left(\frac{n}{2}\right)\left(\frac{m}{2}\right) + \left(\frac{n}{2} - 1\right)\frac{m}{2} = 3mn$$

$$|E(H)| = 2mn$$

$$|E(H^{\star})| = 2mn + \frac{mn}{2} + \left(\frac{n}{2}\right)\left(\frac{m}{2}\right) + \left(\frac{n}{2} - 1\right)\frac{m}{2} + \frac{m}{2} = 3mn$$

$$|V(N^{\star})| = \frac{m(n+1)}{2}$$

and

$$|V(H^{\star})| = \frac{mn}{2}$$

Since $m, n \equiv 0(mod\ 4)$, the graphs N and H are bipartite and starred graphs $N^{\star}$ and $H^{\star}$ are four partite which further implies that $N.\ H \in \mathcal{H}$. Now by using Corollary 2.1, we have:

$$\Delta(N) \leq 2\sqrt{2}$$

and

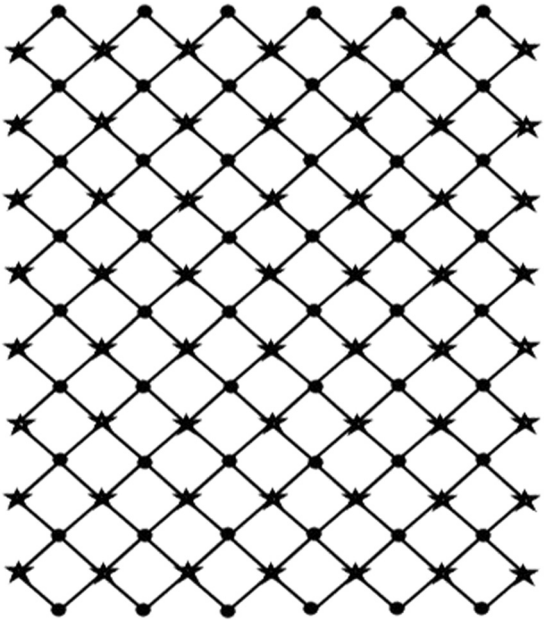

Figure 6: 2D Representation of TUHRC$_4$[6,8] nanotube.

$$\Delta(H) \leq 2\sqrt{2}$$

The 2D-lattice of second family of nanotubes and nanotori is a plane arrangement of C_4 (rhombus). It can either cover a cylinder (nanotube) or a torus (nanotorus). The constructed nanotube is denoted by TUHRC$_4$[m,n], in which m is the number of squares in a row and n is the number of squares in a column as shown in. A 2D representation of TUHRC$_4$[m,n] nanotube and its starred graph are depicted in Figures 6 and 7.

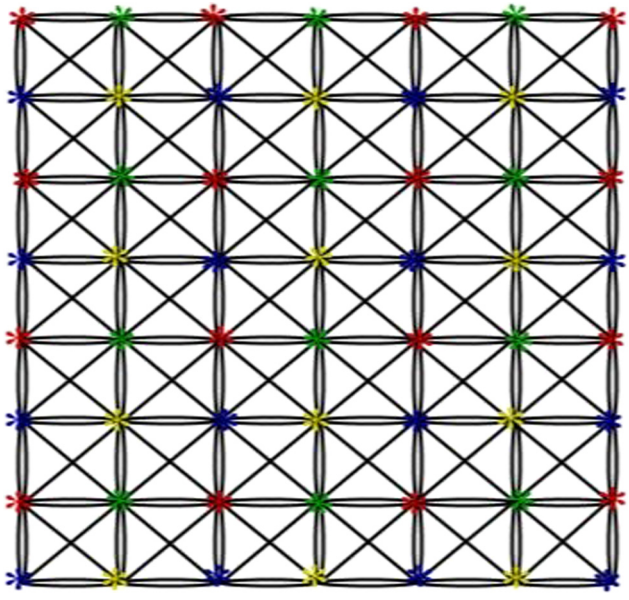

Figure 7: Starred graph G^* of TUHRC$_4$[6,8] nanotube.

Theorem 3.2. *For $m \cdot n > 1$, $m, n \equiv 0(mod\ 2)$, let graphs G_1 and H_1 be molecular graphs of nanotube TUHRC$_4$[m,n] and corresponding nanotorus. Then:*

$$\Delta(N_1) \leq 2\sqrt{3}$$

and

$$\Delta(\mathrm{H}_1) \leq 2\sqrt{3}$$

Proof. Here:

$$|E(G_1)| = 4mn,\ |E(G_1^*)| = 6mn - 4m\ |E(H_1)| = 4mn,$$
$$|E(H_1^*)| = 2m(n-1) + 2(n-1)m + 2m(n-1)$$
$$= 6m(n-1)$$

$$|E(H_1)| = 4mn,$$
$$|E(H_1^*)| = 2m(n-1) + 2(n-1)m + 2m(n-1) = 6m(n-1)$$

and

$$|V(G_1^*)| = mn, |V(H_1^*)| = mn$$

By the same reasoning as used in proof of Theorem 3.1, N_1, $H_1 \in \mathcal{H}$. Hence by Corollary 2.1, $\Delta(N_1) \leq 2\sqrt{3}$ and $\Delta(H_1) \leq 2\sqrt{3}$.

4 Conclusions

The upper bounds of the HOMO–LUMO gap for a special family of bipartite graphs are estimated. The estimated upper bound helps to find the upper bound of the HOMO–LUMO gap for certain nanotubes. In particular, it is shown that the HOMO–LUMO gap for nanotube TUHRC$_4$, and its corresponding nanotorus is found to be $2\sqrt{3}$, and for nanotube TUC$_4$ and its corresponding nanotorus, it is $2\sqrt{2}$. This might be more convenient and helpful in the theoretical study of the molecular orbital theory of nanotubes as compared to Density functional Theory, which only gives programming-based numerical approximations of the HOMO–LUMO gap.

Acknowledgments: The authors are thankful to the referees for their helpful comments and suggestions to improve this article.

Author contributions: Uzma Ahmad: validation, formal analysis, supervision, writing – review; Saira Hameed: writing – original draft, investigation; Ahmed Alamer: funding acquisition; Muhammad Javaid: visualization, validation, proofreading. All authors have read and agreed to the published version of the manuscript.

Conflict of interest: The corresponding author (Muhammad Javaid) is a Guest Editor of the Main Group Metal Chemistry's Special Issue "Theoretical and computational aspects of graph-theoretic methods in modern-day chemistry" in which this article is published.

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