Global and Stochastic Analysis
Vol. 12 No. 2 (March, 2025)

Received: 01st January 2025 *Revised: 19th January 2025* *Accepted: 25th January 2025*

ON MAXIMUM STRESS ENERGY OF GRAPHS

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Abstract. In this article, we introduce the maximum stress matrix $MSM(G)$ for a connected graph G. We investigate the properties of this matrix, establish bounds on its eigenvalues, and define the maximum stress energy $E_{MSM}(G)$ as the sum of the absolute values of its eigenvalues. Furthermore, we discuss its potential relevance in chemistry by comparing $E_{MSM}(G)$ with the π-electron energy of polyaromatic hydrocarbons.

1. Introduction

In this article, we will be focusing on finite, unweighted, simple, and undirected graphs. Let $G = (V, E)$ denote a graph. The degree of a vertex v in G is denoted by $d(v)$. The distance between two vertices u and v in G, denoted $d(u, v)$, is the number of edges in the shortest path (or geodesic) connecting them. A geodesic path P is said to pass through a vertex v if v is an internal vertex of P, meaning v lies on P but is not an endpoint of P. For standard terminology and notion in graph theory, we follow the text-book of Harary [8].

Gutman [6] defined the energy of a graph G as the sum of the absolute values of its eigenvalues, denoted by $\mathcal{E}(G)$. Since eigenvalues have a strong relationship with nearly all of the important graph invariants and extreme properties, they are essential to comprehending graphs. Consequently, graph energy, a specific type of matrix norm, has attracted attention from both pure and applied mathematicians. In order to analyse graph matrices using matrix theory and linear algebra, spectral graph theory—which focusses on matrices related to graphs, particularly their eigenvalues and energies—is essential. Graph energy offers important information about the many dynamic and structural characteristics of graphs. It is a measure that captures the collective influence of a graph's eigenvalues, linking to diverse applications from chemical graph theory to network analysis. Different graph energies associated with topological indices have been introduced and extensively studied in the literature, highlighting their significance in understanding complex systems. Numerous matrices can be related to a graph, and their spectrums provide certain helpful information about the graph [1, 3, 5, 7, 9, 11–14, 21].

2000 *Mathematics Subject Classification.* 05C50, 05C09, 05C92.
Key words and phrases. Graph, Stress of a vertex, Energy, Maximum stress Eigenvalues.
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In 1953, Alfonso Shimbel [23] introduced the notion of vertex stress for graphs as a centrality measure. Stress of a vertex v in a graph G is the number of shortest paths (geodesics) passing through v. This concept has many applications including the study of biological and social networks. Many stress related concepts in graphs and topological indices have been defined and studied by several authors [2, 15–20, 22, 24]. A graph G is k-stress regular [4] if $str(v) = k$ for all $v \in V(G)$.

In this paper, we introduce the maximum stress matrix of a graph G and define the maximum stress energy $E_{MSM}(G)$ based on its eigenvalues. This new approach extends the concept of graph energy to incorporate stress-related measures, offering a fresh perspective on graph invariants. We also establish bounds for $E_{MSM}(G)$ in relation to other graph invariants and explore the correlation between the maximum stress energy of molecules with heteroatoms and their respective π-electron energy. This work aims to deepen our understanding of graph energy and its implications for molecular and structural analysis.

2. Maximum Stress Matrix and Energy

The maximum stress matrix of a graph G with $V(G) = \{v_1, v_2, \cdots, v_n\}$ is defined as $MSM(G) = (x_{ij})$, where

$$x_{ij} = \begin{cases} \max\left(str(v_i), str(v_j)\right), & \text{if} i \neq j; \\ 0, & \text{otherwise} . \end{cases}$$

The maximum stress polynomial of a graph G is defined as

$$P_{MSM(G)}(\lambda_s) = |\lambda_s I - MSM(G)|,$$

where I is an $n \times n$ unit matrix.

All the roots of the equation $P_{MSM(G)}(\lambda_s) = 0$ are real because the matrix $MSM(G)$ is real and symmetric. Therefore, these roots can be ordered as $\lambda_{s_1} \geq \lambda_{s_2} \geq \cdots \geq \lambda_{s_n}$, with λ_{s_1} being the largest and λ_{s_n} being the smallest eigenvalue. The maximum stress energy $E_{MSM}(G)$ of a graph G is defined by

$$E_{MSM}(G) = \sum_{i=1}^{n} |\lambda_{s_i}| .$$

3. Preliminary results

In this section, we will document the necessary results to support our main findings in section 4.

Theorem 3.1. *Let c_i and d_i, for $1 \leq i \leq n$, be non-negative real numbers. Then*

$$\sum_{i=1}^{n} c_i^2 \sum_{i=1}^{n} d_i^2 \leq \frac{1}{4}\left(\sqrt{\frac{M_1M_2}{m_1m_2}} + \sqrt{\frac{m_1m_2}{M_1M_2}}\right)^2 \left(\sum_{i=1}^{n} c_i d_i\right)^2,$$

where $M_1 = \max_{1\leq i\leq n}\{c_i\}; M_2 = \max_{1\leq i\leq n}\{d_i\}; m_1 = \min_{1\leq i\leq n}\{c_i\}$ *and* $m_2 = \min_{1\leq i\leq n}\{d_i\}$.

Theorem 3.2. *Let c_i and d_i, for $1 \le i \le n$ be positive real numbers. Then*

$$\sum_{i=1}^{n} c_i^2 \sum_{i=1}^{n} d_i^2 - \left(\sum_{i=1}^{n} c_i d_i \right)^2 \le \frac{n^2}{4} \left(M_1 M_2 - m_1 m_2 \right)^2,$$

where $M_1 = \max_{1 \le i \le n} \{c_i\}; M_2 = \max_{1 \le i \le n} \{d_i\}; m_1 = \min_{1 \le i \le n} \{c_i\}$ *and* $m_2 = \min_{1 \le i \le n} \{d_i\}$.

Theorem 3.3 (BPR Inequality)**.** *Let c_i and d_i, for $1 \le i \le n$ be non-negative real numbers. Then*

$$\left| n \sum_{i=1}^{n} c_i d_i - \sum_{i=1}^{n} c_i \sum_{i=1}^{n} d_i \right| \le \alpha(n)(A-a)(B-b),$$

where a, b, A and B are real constants, that for each $i, 1 \le i \le n, a \le c_i \le A$ and $b \le d_i \le B$. Further, $\alpha(n) = n \left\lceil \frac{n}{2} \right\rceil \left(1 - \frac{1}{n} \left\lceil \frac{n}{2} \right\rceil \right)$.

Theorem 3.4 (Diaz–Metcalf Inequality)**.** *If c_i and $d_i, 1 \le i \le n$, are nonnegative real numbers, then*

$$\sum_{i=1}^{n} d_i^2 + rR \sum_{i=1}^{n} c_i^2 \le (r+R) \left(\sum_{i=1}^{n} c_i d_i \right),$$

where r and R are real constants, so that for each $i, 1 \le i \le n$, holds $rc_i \le d_i \le Rc_i$.

Theorem 3.5 (The Cauchy-Schwarz inequality)**.** *If $c = (c_1, c_2, \ldots, c_n)$ and $d = (d_1, d_2, \ldots, d_n)$ are real n-vectors, then*

$$\left(\sum_{i=1}^{n} c_i d_i \right)^2 \le \left(\sum_{i=1}^{n} c_i^2 \right) \left(\sum_{i=1}^{n} d_i^2 \right).$$

4. Bounds for the maximum stress Eigenvalues and Energy

Lemma 4.1. *Let $\lambda_{s_1} \ge \lambda_{s_2} \ge \ldots \ge \lambda_{s_n}$ be the eigenvalues of the maximum stress matrix $MSM(G)$. Then*

(i) $\sum_{i=1}^{n} \lambda_{s_i} = 0$

(ii) $\sum_{i=1}^{n} \lambda_{s_i}^2 = 2 \sum_{i<j} \max\left(str(v_i), str(v_j)\right) = 2M_{sm}$,
where $M_{sm} = \sum_{i<j} \max\left(str(v_i), str(v_j)\right)$.

Proof. i) The first equality is a direct consequence of $MSM(G)_{ii} = 0$ for all $1, 2, \ldots, n$.
ii) We have

$$\begin{aligned}\sum_{i=1}^{n} \lambda_{s_i}^2 &= \text{trace}[MSM(G)]^2 \\ &= \sum_{i=1}^{n}\sum_{j=1}^{n} x_{ij}x_{ji} \\ &= \sum_{i=1}^{n} x_{ii}^2 + 2\sum_{i<j} x_{ij}^2 \\ &= 2\sum_{i<j} \max\left(str(v_i), str(v_j)\right) \\ &= 2M_{sm},\end{aligned}$$

where $M_{sm} = \sum_{i<j} \max\left(str(v_i), str(v_j)\right)$

□

Lemma 4.2. *If a, b, c and d are real numbers, then the determinant of the form*
$$\begin{vmatrix} (\lambda+a)\, I_{n\times n} - aJ_{n\times n} & -cJ_{n\times m} \\ -dJ_{m\times n} & (\lambda+b)\, I_{m\times m} - bJ_{m\times m} \end{vmatrix}$$
$$= (\lambda+a)^{n-1}(\lambda+b)^{m-1}\left[(\lambda-(n-1)\,a)(\lambda-(m-1)\,b) - mncd\right].$$

Theorem 4.3. *If $K_{m,n}$ is a complete bipartite graph, then the characteristic polynomial is given by*
$$\left(\lambda_s + \tfrac{n(n-1)}{2}\right)^{m-1}\left(\lambda_s + \tfrac{m(m-1)}{2}\right)^{n-1}$$
$$\times\left[\left(\lambda_s - \tfrac{n(n-1)(m-1)}{2}\right)\left(\lambda_s - \tfrac{m(m-1)(n-1)}{2}\right) - mn\left(\max\left(\tfrac{n(n-1)}{2}, \tfrac{m(m-1)}{2}\right)\right)^2\right].$$

Proof. In a complete bipartite graph $K_{m,n}$, the vertex set $V(K_{m,n})$ can be partitioned into two disjoint sets $A = \{u_1, u_2, ..., u_m\}$ and $B = \{v_1, v_2, ..., v_n\}$. The stress of any vertex v in $K_{m,n}$ is given by

$$Str(v) = \begin{cases} \frac{n(n-1)}{2}, & if\ v \in A; \\ \frac{m(m-1)}{2}, & if\ v \in B. \end{cases}$$

Using the above and the definition of maximum stress matrix, we find that $MSM(K_{m,n}) =$
$$\begin{bmatrix} \frac{n(n-1)}{2}\left(-I_{m\times m} + J_{m\times m}\right) & \max\left(\frac{n(n-1)}{2}, \frac{m(m-1)}{2}\right) J_{m\times n} \\ \max\left(\frac{n(n-1)}{2}, \frac{m(m-1)}{2}\right) J_{n\times m} & \frac{m(m-1)}{2}\left(-I_{n\times n} + J_{n\times n}\right) \end{bmatrix},$$

where I_n is the identity matrix and $J_{n\times m}$ is the matrix with all entries as 1. The characteristic polynomial of the above matrix is given by the following determinant:

$$\begin{vmatrix} \left(\lambda_s + \frac{n(n-1)}{2}\right) I_{m\times m} - \frac{n(n-1)}{2} J_{m\times m} & -\max\left(\frac{n(n-1)}{2}, \frac{m(m-1)}{2}\right) J_{m\times n} \\ & \\ -\max\left(\frac{n(n-1)}{2}, \frac{m(m-1)}{2}\right) J_{n\times m} & \left(\lambda_s + \frac{m(m-1)}{2} I_{n\times n}\right) - \frac{m(m-1)}{2} J_{n\times n} \end{vmatrix}.$$

Using the Lemma 4.2 in the above, we have the characteristic polynomial

$$\left(\lambda_s + \frac{n(n-1)}{2}\right)^{m-1} \left(\lambda_s + \frac{m(m-1)}{2}\right)^{n-1}$$
$$\times \left[\left(\lambda_s - \frac{n(n-1)(m-1)}{2}\right)\left(\lambda_s - \frac{m(m-1)(n-1)}{2}\right) - mn\left(\max\left(\frac{n(n-1)}{2}, \frac{m(m-1)}{2}\right)\right)^2\right].$$

□

Theorem 4.4. *The characteristic polynomial of the cycle C_n is given by*

$$\begin{cases} \left(\lambda_s - \frac{(n-1)^2(n-3)}{8}\right)\left(\lambda_s + \frac{(n-1)(n-3)}{8}\right)^{n-1}, & if\ n\ is\ odd; \\ & \\ \left(\lambda_s - \frac{n(n-1)(n-2)}{8}\right)\left(\lambda_s + \frac{n(n-2)}{8}\right)^{n-1}, & if\ n\ is\ even. \end{cases}$$

Proof. The stress of any vertex v in C_n is given by

$$str(v) = \begin{cases} \frac{(n-1)(n-3)}{8}, & if\ n\ is\ odd; \\ & \\ \frac{n(n-2)}{8}, & if\ n\ is\ even. \end{cases}$$

Using the above and the definition of maximum stress matrix for n being odd, we find that

$$MSM(C_n) = \begin{bmatrix} 0 & \frac{(n-1)(n-3)}{8} & \frac{(n-1)(n-3)}{8} & \cdots & \frac{(n-1)(n-3)}{8} \\ \frac{(n-1)(n-3)}{8} & 0 & \frac{(n-1)(n-3)}{8} & \cdots & \frac{(n-1)(n-3)}{8} \\ \vdots & \vdots & \ddots & \vdots & \\ \frac{(n-1)(n-3)}{8} & \frac{(n-1)(n-3)}{8} & \frac{(n-1)(n-3)}{8} & \cdots & 0 \end{bmatrix}.$$

Using the Lemma 4.2 in the above, the characteristic polynomial of the above matrix is given by

$$\left(\lambda_s - \frac{(n-1)^2(n-3)}{8}\right)\left(\lambda_s + \frac{(n-1)(n-3)}{8}\right)^{n-1}.$$

Again by the definition of maximum stress matrix for n being even, we find that

$$MSM(C_n) = \begin{bmatrix} 0 & \frac{(n)(n-2)}{8} & \frac{(n)(n-2)}{8} & \cdots & \frac{(n)(n-2)}{8} \\ \frac{(n)(n-2)}{8} & 0 & \frac{(n)(n-2)}{8} & \cdots & \frac{(n)(n-2)}{8} \\ \vdots & \vdots & \ddots & \vdots & \\ \frac{(n)(n-2)}{8} & \frac{(n)(n-2)}{8} & \frac{(n)(n-2)}{8} & \cdots & 0 \end{bmatrix}.$$

Using the Lemma 4.2 in the above, the characteristic polynomial of the above matrix is given by

$$\left(\lambda_s - \frac{n(n-1)(n-2)}{8}\right)\left(\lambda_s + \frac{n(n-2)}{8}\right)^{n-1}.$$

□

Theorem 4.5. *Let G be a k-stress regular graph of order n. Then the characteristic polynomial is given by $(\lambda_s - k(n-1))(\lambda_s + k)^{n-1}$.*

Proof. If the graph G is k-stress regular, then $str(v) = k$ for all $v \in V(G)$. Using the definition of maximum stress matrix, we find that

$$MSM(G) = \begin{bmatrix} 0 & k & k & \cdots & k \\ k & 0 & k & \cdots & k \\ \vdots & \vdots & \ddots & \vdots & \\ k & k & k & \cdots & 0 \end{bmatrix}.$$

The characteristic polynomial of the above matrix is given by the following determinant:

$$|\lambda_s I - MSM(G)| = \begin{vmatrix} \lambda_s & -k & -k & \cdots & -k \\ -k & \lambda_s & -k & \cdots & -k \\ \vdots & \vdots & \ddots & \vdots & \\ -k & -k & -k & \cdots & \lambda_s \end{vmatrix}.$$

Using the Lemma 4.2 in the above, we have the characteristic polynomial

$$(\lambda_s - k(n-1))(\lambda_s + k)^{n-1}.$$

□

Theorem 4.6. *If $K_{1\times n-1}$ is a star graph, then the characteristic polynomial is given by*

$$\lambda_s^{n-2}\left[\lambda_s^2 - \frac{(n-1)^3(n-2)^2}{4}\right]$$

Proof. The star graph $K_{1,(n-1)}$ has two types of vertices, namely, internal vertex having stress $\frac{(n-1)(n-2)}{2}$ and remaining vertices having stress 0. Hence,

$$MSM(K_{1\times n-1}) = \begin{bmatrix} (0)_{1\times 1} & \frac{(n-1)(n-2)}{2} J_{1\times(n-1)} \\ \frac{(n-1)(n-2)}{2} J_{(n-1)\times 1} & (0)_{(n-1)\times(n-1)} \end{bmatrix}$$

$$|\lambda_s I - MSM(K_{1\times n-1})| = \begin{vmatrix} \lambda_s I_1 & -\frac{(n-1)(n-2)}{2} J_{1\times(n-1)} \\ -\frac{(n-1)(n-2)}{2} J_{(n-1)\times 1} & \lambda_s I_{(n-1)} \end{vmatrix},$$

where I_r is the identity matrix of order $r\times r$, $0_{m\times m}$ is the zero matrix of order $m\times m$, and $J_{m\times n}$ is the $m\times n$ matrix with all entries equal to 1. Thus, by applying Lemma 4.2, we obtain the desired result. □

Theorem 4.7. *Let G be any graph with n-vertices. Then*

$$\lambda_{s_1} \le \sqrt{\frac{(2M_{sm})(n-1)}{n}}.$$

Proof. Setting $c_i = 1, d_i = \lambda_{s_i}$, for $i = 2, 3, \ldots, n$ in Theorem 3.5, we have

$$\left(\sum_{i=2}^{n} \lambda_{s_i}\right)^2 \le (n-1)\sum_{i=2}^{n} \lambda_{s_i}^2. \tag{4.1}$$

From Lemma 4.1, we find that

$$\sum_{i=2}^{n} \lambda_{s_i} = -\lambda_{s_1} \text{ and } \sum_{i=2}^{n} \lambda_{s_i}^2 = -\lambda_{s_1}^2 + 2M_{sm}.$$

Employing the above in (4.1), we obtain

$$(-\lambda_{s_1})^2 \leq (n-1)\left(2M_{sm} - \lambda_{s_1}^2\right)$$
$$\lambda_{s_1} \leq \sqrt{\frac{(2M_{sm})(n-1)}{n}}.$$

□

Theorem 4.8. *Let G be any graph with n-vertices. Then*

$$E_{MSM}(G) \leq \sqrt{(2M_{sm})n}$$

Proof. Choosing $c_i = 1, d_i = |\lambda_{s_i}|$, for $i = 2, 3, \ldots, n$ in Theorem 3.5, we get

$$\left(\sum_{i=1}^{n} |\lambda_{s_i}|\right)^2 \leq n \sum_{i=1}^{n} \lambda_{s_i}^2$$
$$\Longrightarrow (E_{MSM}(G))^2 \leq n(2M_{sm})$$
$$\Longrightarrow E_{MSM}(G) \leq \sqrt{n(2M_{sm})}.$$

□

Theorem 4.9. *If G is a graph with n vertices and $E_{MSM}(G)$ be the maximum stress energy of G, then*

$$\sqrt{2M_{sm}} \leq E_{MSM}(G).$$

Proof. By the definition of $E_{MSM}(G)$, we have

$$[E_{MSM}(G)]^2 = \left(\sum_{i=1}^{n} |\lambda_{s_i}|\right)^2 \geq \sum_{i=1}^{n} |\lambda_{s_i}|^2 = 2M_{sm}.$$
$$\Longrightarrow \sqrt{2M_{sm}} \leq E_{MSM}(G).$$

□

Theorem 4.10. *Let G be any graph with n-vertices and Φ be the absolute value of the determinant of the maximum stress matrix $MSM(G)$. Then*

$$\sqrt{(2M_{sm}) + n(n-1)\Phi^{2/n}} \leq E_{MSM}(G).$$

Proof. By the definition of maximum stress energy, we find that

$$(E_{MSM}(G))^2 = \left(\sum_{i=1}^{n} |\lambda_{s_i}|\right)^2 = \sum_{i=1}^{n} |\lambda_{s_i}|^2 + 2\sum_{i<j} |\lambda_{s_i}||\lambda_{s_j}|$$

$$= (2M_{sm}) + \sum_{i\neq j} |\lambda_{s_i}||\lambda_{s_j}|.$$

Since for non-negative numbers, the Arithmetic mean is greater than Geometric mean, we have

$$\frac{1}{n(n-1)} \sum_{i\neq j} |\lambda_{s_i}||\lambda_{s_j}| \geq \left(\prod_{i\neq j} |\lambda_{s_i}||\lambda_{s_j}| \right)^{\frac{1}{n(n-1)}}$$
$$= \left(\prod_{i=1}^{n} |\lambda_{s_i}|^{2(n-1)} \right)^{\frac{1}{n(n-1)}}$$
$$= \prod_{i=1}^{n} |\lambda_{s_i}|^{2/n}$$
$$= \Phi^{2/n}.$$

Therefore,

$$\sum_{i\neq j} |\lambda_{s_i}| \left|\lambda_{s_j}\right| \geq n(n-1)\Phi^{\frac{2}{n}}$$
$$\Longrightarrow [E_{MSM}(G)]^2 \geq 2M_{sm} + n(n-1)\Phi^{2/n}$$
$$\Longrightarrow E_{MSM}(G) \geq \sqrt{2M_{sm} + n(n-1)\Phi^{2/n}}.$$

Equality in AM-GM inequality is attained if and only if all $\lambda_{s_i}; i = 1, 2, \ldots, n$ are equal. □

Lemma 4.11. *Let $c_1, c_2, \ldots, c_n$ be non-negative numbers. Then*

$$n\left[\frac{1}{n}\sum_{i=1}^{n} c_i - \left(\prod_{i=1}^{n} c_i\right)^{1/n}\right] \leq n\sum_{i=1}^{n} c_i - \left(\sum_{i=1}^{n} \sqrt{c_i}\right)^2 \leq n(n-1)\left[\frac{1}{n}\sum_{i=1}^{n} c_i - \left(\prod_{i=1}^{n} c_i\right)^{1/n}\right].$$

Theorem 4.12. *Let G be a connected graph with n vertices. Then*

$$\sqrt{(2M_{sm}) + n(n-1)\Phi^{2/n}} \leq E_{MSM}(G) \leq \sqrt{(2M_{sm})(n-1) + n\Phi^{2/n}}.$$

Proof. Let $c_i = |\lambda_{s_i}|^2, i = 1, 2, \ldots, n$ and

$$W = n\left[\frac{1}{n}\sum_{i=1}^{n} |\lambda_{s_i}|^2 - \left(\prod_{i=1}^{n} |\lambda_{s_i}|^2\right)^{1/n}\right]$$
$$= n\left[\frac{(2M_{sm})}{n} - \left(\prod_{i=1}^{n} |\lambda_{s_i}|\right)^{2/n}\right]$$
$$= n\left[\frac{(2M_{sm})}{n} - \Phi^{2/n}\right]$$
$$= (2M_{sm}) - n\Phi^{2/n}.$$

By Lemma 4.11, we obtain

$$W \leq n\sum_{i=1}^{n}|\lambda_{s_i}|^2 - \left(\sum_{i=1}^{n}|\lambda_{s_i}|\right)^2 \leq (n-1)W.$$

Upon simplification of the above equation, we find that

$$\sqrt{(2M_{sm}) + n(n-1)\Phi^{2/n}} \leq E_{MSM}(G) \leq \sqrt{(2M_{sm})(n-1) + n\Phi^{2/n}}.$$

□

Theorem 4.13. *Let G be a graph of order n. Then*

$$E_{MSM}(G) \geq \sqrt{(2M_{sm})n - \frac{n^2}{4}\left(\lambda_{s_1} - \lambda_{s\,\min}\right)^2},$$

where $\lambda_{s_1} = \lambda_{s\,\max} = \max_{1\leq i\leq n}\{|\lambda_{s_i}|\}$ and $\lambda_{s\,\min} = \min_{1\leq i\leq n}\{|\lambda_{s_i}|\}$.

Proof. Suppose $\lambda_{s_1}, \lambda_{s_2}, \ldots, \lambda_{s_n}$ are the eigenvalues of $MSM(G)$. We choose $c_i = 1$ and $d_i = |\lambda_{s_i}|$, which by Theorem 3.2 imply

$$\sum_{i=1}^{n}1^2\sum_{i=1}^{n}|\lambda_{s_i}|^2 - \left(\sum_{i=1}^{n}|\lambda_{s_i}|\right)^2 \leq \frac{n^2}{4}\left(\lambda_{s_1} - \lambda_{s\,\min}\right)^2$$

$$\text{i.e., } (2M_{sm})n - \left(E_{MSM}(G)\right)^2 \leq \frac{n^2}{4}\left(\lambda_{s_1} - \lambda_{s\,\min}\right)^2$$

$$\Longrightarrow E_{MSM}(G) \geq \sqrt{(2M_{sm})n - \frac{n^2}{4}\left(\lambda_{s_1} - \lambda_{s\,\min}\right)^2}.$$

□

Theorem 4.14. *Suppose that zero is not an eigenvalue of $MSM(G)$. Then*

$$(2M_{sm})n \leq \frac{1}{4}\left(\frac{\left(\lambda_{s_1} + \lambda_{s\,\min}\right)^2}{\lambda_{s_1}\lambda_{s\,\min}}\right)\left(E_{MSM}(G)\right)^2,$$

where $\lambda_{s_1} = \lambda_{s\,\max} = \max_{1\leq i\leq n}\{|\lambda_{s_i}|\}$ and $\lambda_{s\,\min} = \min_{1\leq i\leq n}\{|\lambda_{s_i}|\}$.

Proof. Let $\lambda_{s_1}, \lambda_{s_2}, \ldots, \lambda_{s_n}$ be the eigenvalues of $MSM(G)$. Setting $c_i = |\lambda_{s_i}|$ and $d_i = 1$ in Theorem 3.1, we have

$$\sum_{i=1}^{n}|\lambda_{s_i}|^2\sum_{i=1}^{n}1^2 \leq \frac{1}{4}\left(\sqrt{\frac{\lambda_{s_1}}{\lambda_{s\,\min}}} + \sqrt{\frac{\lambda_{s\,\min}}{\lambda_{s_1}}}\right)^2\left(\sum_{i=1}^{n}|\lambda_{s_i}|\right)^2$$

$$\Longrightarrow (2M_{sm})n \leq \frac{1}{4}\left(\frac{\left(\lambda_{s_1} + \lambda_{s\,\min}\right)^2}{\lambda_{s_1}\lambda_{s\,\min}}\right)\left(E_{MSM}(G)\right)^2.$$

□

Theorem 4.15. *Let G be a non-trivial graph . Then $E_{MSM}(G) \geq \sqrt{\frac{(trace(MSM(G)^2))^3}{trace(MSM(G)^4)}}$.*

Proof. Taking $a_i = |\lambda_{s_i}|^{\frac{2}{3}}$, $b_i = |\lambda_{s_i}|^{\frac{4}{3}}$, $p = \frac{3}{2}$ and $q = 3$ in the Holder inequality, we get

$$\sum_{i=1}^{n} |\lambda_{s_i}|^2 = \sum_{i=1}^{n} |\lambda_{s_i}|^{\frac{2}{3}} \left(\left|\lambda_{s_i}^4\right|\right)^{\frac{1}{3}} \leq \left(\sum_{i=1}^{n} |\lambda_{s_i}|\right)^{\frac{2}{3}} \left(\sum_{i=1}^{n} |\lambda_{s_i}|^4\right)^{\frac{1}{3}}.$$

Upon simplification of the above equation, we find that

$$E_{MSM}(G) \geq \left(\frac{\sum_{i=1}^{n} |\lambda_{s_i}|^2}{\left(\sum_{i=1}^{n} |\lambda_{s_i}|^4\right)^{\frac{1}{3}}}\right)^{\frac{3}{2}} = \sqrt{\frac{(trace(MSM(G)^2))^3}{trace(MSM(G)^4)}}.$$

□

Theorem 4.16. *Let G be a graph of order n and $\lambda_{s_1} \geq \lambda_{s_2} \geq \ldots \geq \lambda_{s_n}$ be the non zero eigenvalues of $MSM(G)$. Then*

$$E_{MSM}(G) \geq \frac{(2M_{sm}) + n\lambda_{s_1}\lambda_{s\min}}{\lambda_{s_1} + \lambda_{s\min}},$$

where $\lambda_{s_1} = \lambda_{s\max} = \max_{1\leq i\leq n} \{|\lambda_{s_i}|\}$ and $\lambda_{s\min} = \min_{1\leq i\leq n} \{|\lambda_{s_i}|\}$.

Proof. Assigning $d_i = |\lambda_{s_i}|, c_i = 1, R = |\lambda_{s_1}|$ and $r = |\lambda_{s\min}|$ in Theorem 3.4, we get

$$\begin{aligned} &\sum_{i=1}^{n} |\lambda_{s_i}|^2 + \lambda_{s_1}\lambda_{s\min}\sum_{i=1}^{n} 1^2 \leq (\lambda_{s_1} + \lambda_{s\min})\sum_{i=1}^{n} |\lambda_{s_i}| \\ \Longrightarrow\ &(2M_{sm}) + n\lambda_{s_1}\lambda_{s\min} \leq (\lambda_{s_1} + \lambda_{s\min})\, E_{MSM}(G) \\ \Longrightarrow\ &E_{MSM}(G) \geq \frac{(2M_{sm}) + n\lambda_{s_1}\lambda_{s\min}}{\lambda_{s_1} + \lambda_{s\min}}. \end{aligned}$$

□

Theorem 4.17. *Let G be a graph of order n and $\lambda_{s_1} \geq \lambda_{s_2} \geq \ldots \geq \lambda_{s_n}$ be the eigenvalues of $MSM(G)$. Then*

$$E_{MSM}(G) \geq \sqrt{(2M_{sm})n - \alpha(n)\left(\lambda_{s_1} - \lambda_{s\min}\right)^2},$$

where $\lambda_{s_1} = \lambda_{s\max} = \max_{1\leq i\leq n} \{|\lambda_{s_i}|\}$ and $\lambda_{s\min} = \min_{1\leq i\leq n} \{|\lambda_{s_i}|\}$ and $\alpha(n) = n\left\lceil \frac{n}{2}\right\rceil \left(1 - \frac{1}{n}\left\lceil \frac{n}{2}\right\rceil\right)$.

Proof. Setting $c_i = |\lambda_{s_i}| = d_i, A \leq |\lambda_{s_i}| \leq B$ and $a \leq |\lambda_{s_n}| \leq b$ in Theorem 3.3, we get

$$\begin{aligned} &\left|n\sum_{i=1}^{n} |\lambda_{s_i}|^2 - \left(\sum_{i=1}^{n} |\lambda_{s_i}|\right)^2\right| \leq \alpha(n)\left(\lambda_{s_1} - \lambda_{s\min}\right)^2 \\ \Longrightarrow\ &\left|(2M_{sm})n - (E_{MSM}(G))^2\right| \leq \alpha(n)\left(\lambda_{s_1} - \lambda_{s\min}\right)^2 \\ \Longrightarrow\ &E_{MSM}(G) \geq \sqrt{(2M_{sm})n - \alpha(n)\left(\lambda_{s_1} - \lambda_{s\min}\right)^2}. \end{aligned}$$

□

5. A QSPR Analysis of $E_{MSM}(G)$

In this section, we carry out a computational investigation of the maximum stress energy $E_{MSM}(G)$ and the π-electron energy associated with heteroatoms. The analysis examines quadratic regression models, which are useful for identifying relationships in datasets that display nonlinear characteristics. Given that real-world data often involves such complexity, these regression models offer flexibility in capturing the underlying trends. This section also emphasizes the importance of maximum stress energy in constructing effective quadratic regression model for predicting chemical properties like π-electron energy.

The regression model tested are as follows:
Quadratic equation:

$$Y = A + B_1X + B_2X^2.$$

Here, Y is the dependent variable, A being the regression constant, and B_i (where $i = 1, 2$) are the regression coefficients and X is the independent variable.

TABLE 1. Molecules containing hetero atoms with the maximum stress energy and π-electron energy

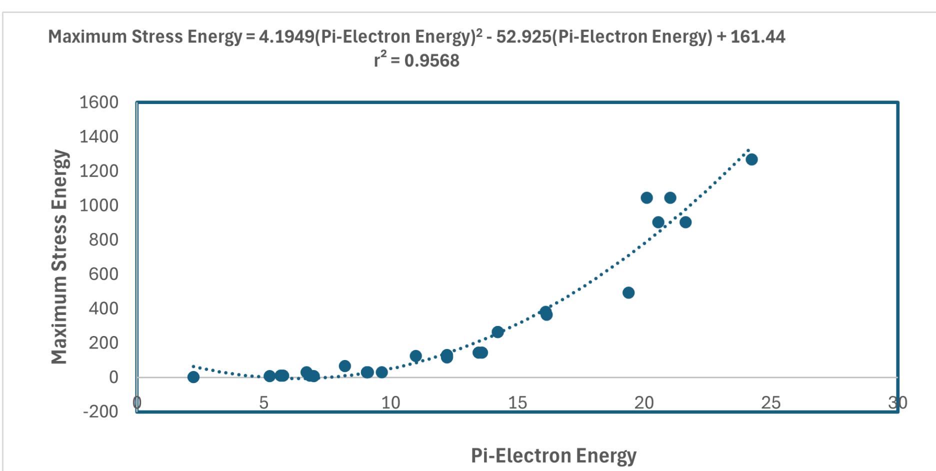
Molecule	$E_{MSM}(G)$	π-electron energy
Veny chloride like system	2.23	2.828
Acrolein like systems	5.76	10.246
1,1-Dichloro-ethylene like systems	6.96	8.485
Glyoxal like and 1,2-Dichloro -ethylene like systems	6.82	10.246
Butadiene perchurbed at C2	5.66	10.246
Pyrrole like systems	5.23	8
Pyridine like systems	6.69	30
Pyridazine like systems	9.06	30
Pyrimidine like systems	9.1	30
Pyrazine like systems	9.07	30
S-Triazene like systems	9.65	30
Aniline like systems	8.19	67.952
O-Phenylene-diamine like systems	12.21	129.788

TABLE 2. Molecules containing hetero atoms with the maximum stress energy and π-electron energy

Molecule	$E_{MSM}(G)$	π-electron energy
m-Phenylene-diamine like systems	12.22	118.055
p-Phenylene-diamine like systems	12.21	123.086
Benzaldehyde like systems	11	126.245
Quinoline like systems	14.23	265.558
Iso-quinoline like systems	14.23	265.558
1-Naphthalein like systems	16.15	364.31
2-Naphthalein like systems	16.12	382.859
Acridine like systems	20.56	902.776
Phenazine like systems	21.62	902.776
Iso-indole like systems	13.46	145.324
Indole like systems	13.59	145.324
Azobenzine like systems	21.02	1046.458
Benzylidine-aniline-like systems	20.1	1046.458
9,10-Anthraquinoline like structures	24.23	1269.925
Cabazole like structures	19.39	494.216

TABLE 3. The correlation coefficient r and r^2 (Adjusted) from quadratic regression model between π electron energy and maximum stress energy

Model	r	r^2
Quadratic Regression Model	0.978	0.9568



6. Conclusion

In conclusion, the maximum stress energy shows considerable promise as a predictor of π-electron energy in chemical compounds. The identified correlation suggests its usefulness in modeling molecular properties, providing a novel method for assessing stability and reactivity. Future research could refine the model's accuracy and broaden its application to a more diverse set of chemical structures.

Acknowledgement. We would like to thank the reviewers for their useful comments and suggestions.

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