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New Bounds on Graph Energy via Topological Indices

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Abstract

This paper establishes a comprehensive framework of novel upper bounds for the energy of graphs, rigorously connecting this spectral invariant to a suite of topological indices. We derive a unified collection of theorems that express graph energy in terms of fundamental parameters—order, size, and extreme degrees—while intricately incorporating advanced indices such as the general zeroth-order Randić index, the Sombor index, and the atom-bond connectivity index. Our results not only generalize but also systematically refine many classical bounds in the literature, demonstrating the profound interplay between spectral graph theory and chemical graph theory.

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1 Introduction

Let $G = (V(G), E(G))$ be a simple undirected graph of order $n = |V(G)|$ and size $m = |E(G)|$. For a vertex $v \in V(G)$, its open neighborhood is denoted by $N_G(v) = \{u \in V(G) \mid uv \in E(G)\}$, and its degree by $d_v = |N_G(v)|$. The degree sequence of G is written in non-increasing order as $(d_1, d_2, \ldots, d_n)$, where $\Delta = d_1$ and $\delta = d_n$ represent the maximum and minimum degrees, respectively. The mean degree is given by $\bar{d} = \frac{2m}{n}$, and the variance of the degrees is defined as:

$$\mathrm{var}(G) = \frac{1}{n} \sum_{v \in V(G)} \left(d_v - \bar{d}\right)^2 .$$

A graph is connected if every pair of distinct vertices is joined by a path. The distance $d(u, w)$ between vertices u and w is the length of a shortest path connecting them, and the diameter $\mathrm{diam}(G)$ is the maximum distance over all vertex pairs. A matching is a set of edges without common vertices, and the matching number $\vartheta(G)$ is the size of a maximum matching.

Topological indices are numerical invariants that capture structural features of graphs and have found extensive applications in mathematical chemistry. Among the most studied is the Wiener index, defined as the sum of distances between all vertex pairs, which correlates with physicochemical properties such as boiling points and molecular volumes ([13, 30, 36]).

The Randić index, introduced in [31], is defined as:

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}},$$

and has been linked to molecular stability and biological activity [8]. A generalization, the general zeroth-order Randić index, is given by:

$$^0R_\alpha(G) = \sum_{v \in V(G)} d_v^\alpha,$$

where $\alpha \in \mathbb{R}$. Special cases include the inverse index $ID(G) = {}^0R_{-1}(G)$, the first Zagreb index $M_1(G) = {}^0R_2(G)$, and the forgotten index $F(G) =$

${}^0R_3(G)$.

The general Randić index extends this concept to edges:

$$R_\alpha(G) = \sum_{uv \in E(G)} (d_u d_v)^\alpha.$$

For $\alpha = -\frac{1}{2}$, it reduces to the classical Randić index.

Zagreb indices, introduced in [14], are defined as:

$$M_1(G) = \sum_{v \in V(G)} d_v^2, \quad M_2(G) = \sum_{uv \in E(G)} d_u d_v,$$

and have been widely used to estimate molecular energy and stability [4, 33].

Recent years have seen the introduction of several new indices. The Sombor index [18] is defined as:

$$SO(G) = \sum_{uv \in E(G)} \sqrt{d_u^2 + d_v^2}.$$

The atom-bond connectivity (ABC) index [10] is given by:

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}},$$

and has been applied to predict properties of organic compounds [5, 10]. The general sum-connectivity index [39] is:

$$X_\alpha(G) = \sum_{uv \in E(G)} (d_u + d_v)^\alpha,$$

with the sum-connectivity index $SCI(G) = X_{-1/2}(G)$ introduced in [38]. The first general multiplicative Zagreb index [35] is:

$$P^\alpha(G) = \prod_{v \in V(G)} d_v^\alpha,$$

which generalizes the Narumi–Katayama index $NK(G) = P^1(G)$ [29].

The adjacency matrix $A(G)$ of G has entries $a_{ij} = 1$ if $v_iv_j \in E(G)$, and 0 otherwise. Its eigenvalues are denoted $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$, where λ_1 is the spectral radius. The energy of G is defined as:

$$\mathcal{E}(G) = \sum_{i=1}^{n} |\lambda_i|,$$

and was introduced by Gutman [15] in the context of Hückel molecular orbital theory to approximate the total π-electron energy of conjugated hydrocarbons [14, 16, 17].

While numerous inequalities have been established for graph energy and topological indices individually, results connecting the two are relatively scarce [3, 37]. Recent work by Filipovski [11] derived relations between energy and other graph parameters. Ülker, Gürsoy, Gürsoy ([34]) showed that $\mathcal{E}(G) \leq SO(G)$ for graphs with $\delta \geq 2$, and $\mathcal{E}(G) \leq (SO(G))^2$ for regular graphs. Yan, Liu, Pan, Li ([37]) proved that $\mathcal{E}(G) \leq 2\sqrt{\Delta}R(G)$, and Gutman, Monsalve, Rada ([19]) obtained relations between vertex-degree-based indices and energy.

In this paper, we establish new and refined bounds connecting graph energy with various topological indices, including the general zeroth-order Randić index, general sum-connectivity index, Sombor index, classical Randić index, Narumi–Katayama index, sum-connectivity index, and atom-bond connectivity index. Section 2 presents preliminary results, and Section 3 contains our main theorems.

2 Preliminaries

This section presents fundamental results on graph energy and the general zeroth-order Randić index from the literature, along with essential analytical inequalities required for our main proofs.

Theorem 1 ([34]). *Let G be a graph.*

(i) If $\delta(G) \geq 2$, then $\mathcal{E}(G) \leq SO(G)$.

(ii) If G is regular, then $\mathcal{E}(G) \leq (SO(G))^2$, with equality if and only if $G \cong K_2$.

The following theorems establish important bounds for the general zeroth-order Randić index:

Theorem 2 ([20]). *Let G be a graph of order n. Then*

$$^{0}R_{-\frac{1}{2}}(G) \geq \sqrt{^{0}R_{-1}(G) + 2R(G)},$$

with equality if and only if $G \cong K_n$.

Theorem 3 ([6]). *Let G be a connected graph of order n with maximum degree Δ. Then*

$$^{0}R_{-\frac{1}{2}}(G) \geq \frac{2\sqrt{2}SCI(G)}{\Delta},$$

with equality if and only if G is regular.

Theorem 4 ([21]). *If T is a tree with $n \geq 2$ vertices and matching number $\vartheta(T)$, then*

$$^{0}R_{-1}(T) \leq \frac{5}{4}n - \frac{1}{2} + \frac{2}{n} - \vartheta(T).$$

Theorem 5 ([20]). *Let G be a graph of order $n \geq 2$. Then*

$$^{0}R_{-1}(G) \leq \left(\frac{2m}{n}\right)^{n-1} \frac{n}{NK(G)}.$$

Proposition 6 ([28]). *If G is a graph of order n and diameter* diam(G)*, then*

$$^{0}R_{-1}(G) \leq \frac{3n}{2} - \mathrm{diam}(G).$$

Theorem 7 ([7]). *Let G be a graph of order n with no isolated vertices. If $\delta \geq 2$, then*

$$^{0}R_{-1}(G) < ABC(G).$$

Classical bounds for graph energy include:

Theorem 8 ([22]). *Let G be a graph with n vertices and m edges. Then*

$$\mathcal{E}(G) \leq \sqrt{2mn}. \tag{1}$$

Theorem 9 ([2]). *For a graph G with vertices $v_1, \ldots, v_n$ having degrees $d_1, \ldots, d_n$, we have*

$$\mathcal{E}(G) \leq \sum_{i=1}^{n} \sqrt{d_i} \leq \sqrt{2mn}, \tag{2}$$

where the second inequality holds if and only if G is regular.

We now recall several analytical inequalities essential for our derivations:

Lemma 1 ([12]). *Let $a_1, \ldots, a_n$ be positive real numbers with $\sum a_i^2 \neq 0$. Then*

$$\sqrt{\frac{\sum a_i^2}{n}} \geq \frac{\sum a_i}{n} + \frac{1}{4n} \sum_{i=1}^{n} \frac{(na_i^2 - \sum a_j^2)^2}{n^2 a_i^4 + (\sum a_j^2)^2} a_i. \tag{3}$$

Lemma 2 ([9]). *Let $x_1, \ldots, x_n$ be non-negative numbers, and $\alpha, \beta \in [1, \infty)$ with $\alpha \leq \beta$. Then*

$$\left(\sum_{i=1}^{n} x_i^{\alpha} \right)^{\frac{\beta}{\alpha}} \leq n^{\frac{\beta}{\alpha} - 1} \left(\sum_{i=1}^{n} x_i^{\beta} \right). \tag{4}$$

Lemma 3 ([9]). *Let $x_1, \ldots, x_n$ be non-negative numbers, and k a positive integer. Then*

$$\left(\sum_{i=1}^{n} x_i \right) \left(\sum_{i=1}^{n} x_i^{k-1} \right) \leq n \left(\sum_{i=1}^{n} x_i^{k} \right). \tag{5}$$

Lemma 4 ([25, 27]). *Let $p = (p_i)$ and $a = (a_i)$, $i = 1, 2, \ldots, n$, be sequences of non-negative and positive real numbers, respectively. For any $r \leq 0$ or $r \geq 1$,*

$$\left(\sum_{i=1}^{n} p_i \right)^{r-1} \sum_{i=1}^{n} p_i a_i^r \geq \left(\sum_{i=1}^{n} p_i a_i \right)^{r}. \tag{6}$$

The reverse inequality holds when $0 \leq r \leq 1$. Equality occurs if and only if either $r = 0$, $r = 1$, $a_1 = \cdots = a_n$, or the sequences p and a have specific zero patterns.

Lemma 5 ([24]). *Let $a = (a_i)$, $i = 1, \dots, n$, be a real sequence with $0 < r \le a_i \le R < \infty$. Then*

$$\sum_{j=1}^{n} a_j \sum_{j=1}^{n} \frac{1}{a_j} \le n^2 \left[1 + \frac{1}{4}\left(1 - \frac{1+(-1)^{n+1}}{2n^2}\right)\left(\sqrt{\frac{R}{r}} - \sqrt{\frac{r}{R}}\right)^2 \right]. \quad (7)$$

Lemma 6 ([26]). *If $a_k, b_k \in \mathbb{R}$ for $k = 1, \dots, n$, and $\frac{1}{p} + \frac{1}{q} = 1$ with $p > 1$, then*

$$\left(\sum_{k=1}^{n} |a_k|^p\right)^{1/p} \left(\sum_{k=1}^{n} |b_k|^q\right)^{1/q} \ge \sum_{k=1}^{n} |a_k b_k|. \quad (8)$$

We now prove a key monotonicity property:

Lemma 7. *Let G be a graph of order n, size m and minimum degree $\delta \ge 1$. Then for any real number $r \ge 0$, $\sqrt[r+1]{(2m)^r\, {}^0R_{\frac{1-r}{2}}(G)}$ is non-decreasing in r.*

Proof. Let $y_i = \sqrt{d_i}$ so that $y_i^2 = d_i$. Consider integer numbers r_1, r_2 such that $r_1 > r_2 \ge 0$ and define

$$F(r) = \left(\sum_{i=1}^{n} y_i^2\right)^{\frac{r}{r+1}} \left(\sum_{i=1}^{n} y_i^{1-r}\right)^{\frac{1}{r+1}}. \quad (9)$$

Note that $1 - r_2 = \dfrac{r_2+1}{r_1+1}(1 - r_1) + 2\left(1 - \dfrac{r_2+1}{r_1+1}\right)$. Let $\theta \in (0,1)$ be defined by $\theta = \dfrac{r_2+1}{r_1+1}$. Then $1 - r_2 = \theta(1 - r_1) + 2(1 - \theta)$. Moreover, $y_i^{1-r_2} = \left(y_i^{1-r_1}\right)^{\theta} \left(y_i^2\right)^{1-\theta}$, which implies

$$\sum_{i=1}^{n} y_i^{1-r_2} = \sum_{i=1}^{n} \left(y_i^{1-r_1}\right)^{\theta} \left(y_i^2\right)^{1-\theta}.$$

Applying Lemma 6 for $a_i = y_i^{1-r_1}$, $b_i = y_i^2$, $p = \dfrac{1}{\theta}$, and $q =$

$\dfrac{1}{1-\theta}$, we have that

$$\sum_{i=1}^{n} y_i^{1-r_2} = \sum_{i=1}^{n} \left(y_i^{1-r_1}\right)^{\theta} \left(y_i^2\right)^{1-\theta} \leq \left(\sum_{i=1}^{n} y_i^{1-r_1}\right)^{\theta} \left(\sum_{i=1}^{n} y_i^2\right)^{1-\theta}.$$

Raising both sides to the power r_1+1, we have

$$\left(\sum_{i=1}^{n} y_i^{1-r_2}\right)^{r_1+1} \leq \left(\sum_{i=1}^{n} y_i^{1-r_1}\right)^{\theta(r_1+1)} \left(\sum_{i=1}^{n} y_i^2\right)^{(1-\theta)(r_1+1)}.$$

It follows that

$$\left(\sum_{i=1}^{n} y_i^{1-r_2}\right)^{r_1+1} \leq \left(\sum_{i=1}^{n} y_i^{1-r_1}\right)^{r_2+1} \left(\sum_{i=1}^{n} y_i^2\right)^{r_1-r_2}.$$

Dividing both sides by $\left(\sum_{i=1}^{n} y_i^{1-r_2}\right)^{r_1+1}$, we get

$$1 \leq \frac{\left(\sum_{i=1}^{n} y_i^{1-r_1}\right)^{r_2+1} \left(\sum_{i=1}^{n} y_i^2\right)^{r_1-r_2}}{\left(\sum_{i=1}^{n} y_i^{1-r_2}\right)^{r_1+1}}.$$

Taking the $(r_1+1)-$th root from both sides

$$1 \leq \frac{\left(\sum_{i=1}^{n} y_i^{1-r_1}\right)^{\frac{r_2+1}{r_1+1}} \left(\sum_{i=1}^{n} y_i^2\right)^{\frac{r_1-r_2}{r_1+1}}}{\sum_{i=1}^{n} y_i^{1-r_2}}.$$

Now, taking the $(r_2+1)-$th root from both sides and after multiplying it by $\dfrac{\left(\sum_{i=1}^{n} y_i^2\right)^{\frac{r_2}{r_2+1}}}{\left(\sum_{i=1}^{n} y_i^2\right)^{\frac{r_2}{r_2+1}}}$, we have

$$1 \leq \frac{\left(\sum_{i=1}^{n} y_i^{1-r_1}\right)^{\frac{1}{r_1+1}} \left(\sum_{i=1}^{n} y_i^2\right)^{\frac{r_1-r_2}{(r_1+1)(r_2+1)}}}{\left(\sum_{i=1}^{n} y_i^{1-r_2}\right)^{\frac{1}{r_2+1}}} =$$

$$\frac{\left(\sum_{i=1}^{n} y_i^{1-r_1}\right)^{\frac{1}{r_1+1}} \left(\sum_{i=1}^{n} y_i^2\right)^{\frac{r_1-r_2}{(r_1+1)(r_2+1)}} \left(\sum_{i=1}^{n} y_i^2\right)^{\frac{r_2}{r_2+1}}}{\left(\sum_{i=1}^{n} y_i^{1-r_2}\right)^{\frac{1}{r_2+1}} \left(\sum_{i=1}^{n} y_i^2\right)^{\frac{r_2}{r_2+1}}}.$$

After some algebraic manipulation, it follows that

$$1 \leq \frac{\left(\sum_{i=1}^{n} y_i^{1-r_1}\right)^{\frac{1}{r_1+1}} \left(\sum_{i=1}^{n} y_i^2\right)^{\frac{r_1}{r_1+1}}}{\left(\sum_{i=1}^{n} y_i^{1-r_2}\right)^{\frac{1}{r_2+1}} \left(\sum_{i=1}^{n} y_i^2\right)^{\frac{r_2}{r_2+1}}} = \frac{F(r_1)}{F(r_2)},$$

$$\Leftrightarrow F(r_2) \leq F(r_1)$$

From Equation (9) and replacing the values y_i^2 and y_i the result follows. ■

Remark. From Lemma 7 and Theorem 9 for $r \geq 0$, we have

$$\mathcal{E}(G) \leq \sum_{i=1}^{n} \sqrt{d_i} \leq \sqrt[r+1]{(2m)^r \, {}^0R_{\frac{1-r}{2}}(G)}. \tag{10}$$

3 Main results

This section presents our principal contributions, establishing new relationships between graph energy and various topological indices. We begin with a result connecting energy to degree variance and extremal degrees.

Theorem 10. *Let G be a graph of order n with $m \geq 1$ edges, maximum degree Δ, minimum degree δ, and the variance of degrees $var(G)$. Then*

$$\mathcal{E}(G) \leq \sqrt{2mn} - \frac{n\sqrt{\delta}var(G)}{8\Delta^2}. \tag{11}$$

If the equality is attained, then G is a regular graph.

Proof. Making $a_i = \sqrt{d_i}$ for $i = 1, 2, \ldots, n$ in inequality (1), we have

$$\sqrt{\frac{d_1 + \cdots + d_n}{n}} \geq \frac{\sqrt{d_1} + \cdots + \sqrt{d_n}}{n} + \frac{1}{4n}\sum_{i=1}^{n} \frac{(nd_i - (d_1 + \cdots + d_n))^2}{n^2 d_i^2 + (d_1 + \cdots + d_n)^2}\sqrt{d_i} \tag{12}$$

$$\geq \frac{\sqrt{d_1} + \cdots + \sqrt{d_n}}{n} + \frac{\sqrt{\delta}}{4n}\sum_{i=1}^{n} \frac{(d_i - (\frac{2m}{n}))^2}{d_i^2 + (\frac{2m}{n})^2} \tag{13}$$

$$\geq \frac{\sqrt{d_1} + \cdots + \sqrt{d_n}}{n} + \frac{\sqrt{\delta}}{4n}\sum_{i=1}^{n} \frac{(d_i - (\frac{2m}{n}))^2}{\Delta^2 + \Delta^2} \tag{14}$$

$$= \frac{\sqrt{d_1} + \cdots + \sqrt{d_n}}{n} + \frac{\sqrt{\delta}var(G)}{8\Delta^2} \tag{15}$$

So

$$\sqrt{2mn} - \frac{n\sqrt{\delta}var(G)}{8\Delta^2} \geq \sqrt{d_1} + \cdots + \sqrt{d_n} \tag{16}$$

and from Theorem 9, the inequality (11) follows.

Now suppose that the equality holds in (11). Then all the inequalities in the proof must be equalities. From the equalities (13) and (14), we have $d_i^2 = \Delta^2$ for $i = 1, 2, \ldots, n$ and $\left(\frac{2m}{n}\right)^2 = \Delta^2$, i.e., G is a regular graph. ■

Remark. Table 1 shows that the bound (11) improves McClelland's classical bound (1) for irregular graphs, while equality is recovered in the regular case. This numerical behavior is consistent with the analytical expression of (11), since the correction term $\frac{n\sqrt{\delta}\,\mathrm{var}(G)}{8\Delta^2}$ is non-negative, yielding a strictly better bound whenever $\mathrm{var}(G)$[†] > 0.

[†] Variance of the degrees of graph G.

Table 1. Numerical comparison between McClelland's bound (Theorem 8) and the improved bound presented on Theorem 10 for some graphs.

Graph G	n	$\mathcal{E}(G)$	Theorem 8	Theorem 10
P_{10} (Path)	10	12.20	13.42	13.29
C_{10} (Cycle)	10	12.94	14.14	14.14
S_{10} (Star)	10	6.00	13.42	11.48
$K_{3,3}$	6	6.00	8.49	7.07
$K_{4,6}$	10	9.80	15.49	12.87
Benzene (C_6)	6	8.00	8.49	8.49
Naphthalene	10	13.70	14.83	14.05
Anthracene	14	19.31	20.98	19.67
Phenanthrene	14	19.31	20.98	19.42

The next result presents an upper bound for the energy of graphs in terms of order, maximum degree, and general zeroth-order Randić index of graphs.

Theorem 11. *Let G be a graph of order $n \geq 3$ without isolated vertices. Then, for any real number $\beta \geq 2$, we have that*

$$\mathcal{E}(G) \leq \sqrt{\Delta} + (n-1)^{\frac{\beta-2}{\beta}} \left({}^0R_{\frac{\beta}{4}} - \Delta^{\frac{\beta}{4}} \right)^{\frac{2}{\beta}} . \tag{17}$$

If $G \cong nK_1$, the equality holds.

Proof. Making $x_i = \sqrt[4]{d_i}$ for $i = 2, 3, \ldots, n$ and $\alpha = 2$ in inequality (2) we have

$$\left(\sum_{i=2}^{n} \sqrt{d_i} \right)^{\frac{\beta}{2}} \leq (n-1)^{\frac{\beta}{2}-1} \left(\sum_{i=2}^{n} d_i^{\frac{\beta}{4}} \right)$$

that is,

$$\sum_{i=2}^{n} \sqrt{d_i} \leq \left((n-1)^{\frac{\beta-2}{2}} \sum_{i=2}^{n} d_i^{\frac{\beta}{4}} \right)^{\frac{2}{\beta}} \tag{18}$$

$$= (n-1)^{\frac{\beta-2}{\beta}} \left(\sum_{i=2}^{n} d_i^{\frac{\beta}{4}} \right)^{\frac{2}{\beta}} . \tag{19}$$

From Theorem 9, Inequality (19), and the definition of zeroth-order Randić index of graphs, the result follows. If $G \cong nK_1$, it is easy to see that the equality holds. ■

Remark. For $\beta = 4$ and from inequality (17) we have $\mathcal{E}(G) \leq \sqrt{\Delta} + \sqrt{(n-1)(2m-\Delta)}$ which was proven in [1] and [23]. So, this bound is a particular case of Theorem 11.

Using the same technique of the proof presented in Theorem 11, we obtain the next two results.

Theorem 12. *Let G be a graph of order $n \geq 3$ without isolated vertices. Then, for any real number $\beta \geq 2$, we have that*

$$\mathcal{E}(G) \leq \sqrt{\Delta} + \sqrt{\delta} + (n-2)^{\frac{\beta-2}{\beta}} \left({}^0R_{\frac{\beta}{4}} - \Delta^{\frac{\beta}{4}} - \delta^{\frac{\beta}{4}} \right)^{\frac{2}{\beta}} . \tag{20}$$

Theorem 13. *Let G be a graph of order $n \geq 3$. Then, for any real number $\beta \geq 2$, we have that*

$$\mathcal{E}(G) \leq n^{\frac{\beta-2}{\beta}} \left({}^0R_{\frac{\beta}{4}} \right)^{\frac{2}{\beta}} . \tag{21}$$

For $\beta = 4$, we have the following corollary of Theorem 12 which can be seen in [11].

Corollary. *([11]) Let G be a graph of order $n \geq 3$ with m, maximum degree Δ, and minimum degree δ. Then*

$$\mathcal{E}(G) \leq \sqrt{\Delta} + \sqrt{\delta} + \sqrt{(n-2)(2m-\Delta-\delta)}.$$

Remark. For $\beta = 4$ in Theorem 13, we obtain Theorem 8, while for $\beta = 8$ and $\beta = 12$, also in Theorem 13, we have the bounds $\mathcal{E}(G) \leq \sqrt[4]{n^3 M_1(G)}$ and $\mathcal{E}(G) \leq \sqrt[6]{n^5 F(G)}$, respectively.

The next result gives a relationship between the energy and the general sum-connectivity index of graphs.

Theorem 14. *Let G be a graph of order n with minimum degree $\delta \geq 1$. Then*

$$\mathcal{E}(G) \leq \frac{\sqrt{2} X_{\frac{1}{2}}(G)}{\delta}. \tag{22}$$

The equality holds if $G \cong \frac{n}{2}K_2$, *for* n *even, or* G *is a graph with no edge.*

Proof. Consider the function $f(x) = x^\alpha$ for $x > 0$, with $0 < \alpha < 1$. If $0 < \alpha < 1$, then f is convex and

$$\left(\frac{d_u + d_v}{2}\right)^\alpha \geq \frac{d_u^\alpha + d_v^\alpha}{2}$$

that is,

$$d_u^\alpha + d_v^\alpha \leq 2^{1-\alpha}\left(d_u + d_v\right)^\alpha .$$

Making $\alpha = \frac{1}{2}$ in the above inequality, we have

$$\sqrt{d_u} + \sqrt{d_v} \leq \sqrt{2\left(d_u + d_v\right)}. \tag{23}$$

From inequality (23) and Theorem 9, we have

$$\mathcal{E}(G) \leq \sum_{v \in V(G)} \sqrt{d_v} = \sum_{uv \in E(G)} \left(\frac{1}{\sqrt{d_u}} + \frac{1}{\sqrt{d_v}}\right) \tag{24}$$

$$= \sum_{uv \in E(G)} \frac{\sqrt{d_u} + \sqrt{d_v}}{\sqrt{d_u d_v}}$$

$$\leq \sum_{uv \in E(G)} \frac{\sqrt{2\left(d_u + d_v\right)}}{\sqrt{d_u d_v}} \tag{25}$$

$$\leq \frac{\sqrt{2} X_{\frac{1}{2}}(G)}{\delta}, \tag{26}$$

and the bound follows. If $G \cong \frac{n}{2}K_2$, for n even, or G is a graph with no edge, it is easy to see that the equality holds. ■

Remark. From inequality (25), we have

$$\mathcal{E}(G) \leq \sum_{uv \in E(G)} \frac{\sqrt{2\left(d_u + d_v\right)}}{\sqrt{d_u d_v}} \leq \sum_{uv \in E(G)} \frac{2\sqrt{\Delta}}{\sqrt{d_u d_v}} = 2\sqrt{\Delta} R(G),$$

which was proved in [37].

Remark. From Theorem 14, we have

$$\mathcal{E}(G) \leq \sum_{uv\in E(G)} \frac{\sqrt{2}X_{\frac{1}{2}}(G)}{\delta} = \sum_{uv\in E(G)} \frac{\sqrt{2\,(d_u + d_v)}}{\delta}$$
$$\leq \sum_{uv\in E(G)} \frac{\sqrt{2\,(d_u^2 + d_v^2)}}{\delta} = \frac{\sqrt{2}SO(G)}{\delta}.$$

Table 2 shows that the bound provided by Theorem 14 is consistently sharper than that of Theorem 1 for all considered graphs with $\delta \geq 2$. In particular, the improvement is clearly visible for classical benzenoid graphs such as benzene, naphthalene, anthracene, pyrene, and coronene, highlighting the relevance of the proposed bound in chemical graph theory.

Table 2. Numerical comparison between the upper bounds given in Theorem 14 and Theorem 1 for graphs with minimum degree $\delta \geq 2$.

Graph G	δ	$\mathcal{E}(G)$	Theorem 14	Theorem 1
$K_{4,4}$	4	8.00	16.01	64.00
K_5	4	8.00	11.31	28.28
Q_3 (cube)	3	8.00	13.07	33.94
Benzene (C_6)	2	8.00	9.49	18.97
Naphthalene	2	13.70	20.90	41.81
Anthracene	2	19.31	31.62	63.25
Pyrene	2	18.49	28.28	56.57
Coronene	2	36.00	50.91	101.82

Remark. For some graph G such that $\delta \geq 1$ we have,

$$\sqrt{2} \leq \delta SO(G) \Leftrightarrow \frac{\sqrt{2}SO(G)}{\delta} \leq (SO(G))^2$$

and from Remark 3, it follows

$$\mathcal{E}(G) \leq \sum_{uv\in E(G)} \frac{\sqrt{2}X_{\frac{1}{2}}(G)}{\delta} \leq \frac{\sqrt{2}SO(G)}{\delta} \leq (SO(G))^2.$$

As a consequence, the bound in Theorem 14 is sharper than that in Theorem 1 for regular graphs. In addition, Table 2 also includes the regular graphs K_5 and Q_3, illustrating the performance of the proposed bound on regular, non-cyclic structures.

The next result presents a bound for the energy of a graph as a function of the number of edges and the degrees of the graph.

Proposition 15. *Let G be a graph of order $n \geq 2$ and size m. Then*

$$\mathcal{E}(G) \leq \sqrt{2m + 2 \sum_{1 \leq i < j \leq n} \sqrt{d_i d_j}}. \tag{27}$$

If $G \cong \overline{K}_n$, the equality holds.

Proof. We know that

$$\left(\sum_{i=1}^{n} \sqrt{d_1} \right)^2 = \sum_{i=1}^{n} d_i + 2 \sum_{1 \leq i < j \leq n} \sqrt{d_i d_j} = 2m + 2 \sum_{1 \leq i < j \leq n} \sqrt{d_i d_j}.$$

From Theorem 9, we have

$$\mathcal{E}(G) \leq \sum_{i=1}^{n} \sqrt{d_1} = \sqrt{2m + 2 \sum_{1 \leq i < j \leq n} \sqrt{d_i d_j}},$$

proving the inequality. If $G \cong \bar{K}_n$, the equality holds. ■

Remark. It is easy to see that

$$\sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \left(\sqrt{d_i} - \sqrt{d_j} \right)^2 = (n-1) \sum_{i=1}^{n} d_i - 2 \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \sqrt{d_i d_j}. \tag{28}$$

As $\sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \left(\sqrt{d_i} - \sqrt{d_j} \right)^2 \geq 0$ and $\sum_{i=1}^{n} d_i = 2m$, from equality (28), we conclude that

$$2 \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \sqrt{d_i d_j} \leq 2m(n-1).$$

Moreover, from Proposition 15, we get

$$\mathcal{E}(G) \leq \sqrt{2m + 2\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}\sqrt{d_i d_j}} \leq \sqrt{2m + 2m(n-1)} = \sqrt{2mn}.$$

Therefore, the bound given in Proposition 15 is sharper than that of Theorem 8. Table 3 numerically illustrates this improvement for all tested irregular graphs, while both bounds coincide in the regular case. The improvement is particularly pronounced for graphs with highly non-uniform degree distributions, such as stars and chemical graphs.

Table 3. Numerical comparison between the upper bounds given in Proposition 15 and Theorem 8 for some graphs.

Graph G	n	m	$\mathcal{E}(G)$	Theorem 8	Proposition 15
P_{10}	10	9	12.05	13.42	13.31
C_{10}	10	10	12.94	14.14	14.14
$S_{10} = K_{1,9}$	10	9	6.00	13.42	12.00
$K_{4,4}$	8	16	8.00	16.00	16.00
$K_{4,6}$	10	24	9.80	21.91	21.80
Benzene (C_6)	6	6	8.00	8.49	8.49
Naphthalene	10	11	13.68	14.83	14.78
Anthracene	14	16	19.45	21.17	21.07
Phenanthrene	14	16	19.31	21.17	21.07

The next result presents an upper bound for the energy of a graph as a function of the maximum degree, minimum degree, and the general zeroth-order Randić index of the graph.

Proposition 16. *Let G be a connected graph of order n, with maximum degree Δ and minimum degree $\delta \geq 1$. Then*

$$\mathcal{E}(G) \leq \frac{n^2\left[1 + \frac{1}{4}\left(1 - \frac{1+(-1)^{n+1}}{2n^2}\right)\left(\sqrt[4]{\frac{\Delta}{\delta}} - \sqrt[4]{\frac{\delta}{\Delta}}\right)^2\right]}{{}^0R_{-\frac{1}{2}}(G)}. \tag{29}$$

Proof. Making $a_i = \sqrt{d_i}$ for $i = 1, 2, \ldots n$, $R = \sqrt{\Delta}$ and $r = \sqrt{\delta}$ in

Inequality (5), we have

$$\sum_{i=1}^{n}\sqrt{d_i}\sum_{i=1}^{n}\frac{1}{\sqrt{d_i}} \le n^2\left[1+\frac{1}{4}\left(1-\frac{1+(-1)^{n+1}}{2n^2}\right)\left(\sqrt[4]{\frac{\Delta}{\delta}}-\sqrt[4]{\frac{\delta}{\Delta}}\right)^2\right] \tag{30}$$

and consequently

$$\sum_{i=1}^{n}\sqrt{d_i} \le \frac{n^2\left[1+\frac{1}{4}\left(1-\frac{1+(-1)^{n+1}}{2n^2}\right)\left(\sqrt[4]{\frac{\Delta}{\delta}}-\sqrt[4]{\frac{\delta}{\Delta}}\right)^2\right]}{\sum_{i=1}^{n}\frac{1}{\sqrt{d_i}}}. \tag{31}$$

From (31) and Theorem 9, the claim follows. ■

Remark. Applying the harmonic mean and quadratic mean inequalities to the positive numbers $\frac{1}{\sqrt{d_1}}, \frac{1}{\sqrt{d_2}}, \ldots, \frac{1}{\sqrt{d_n}}$, we obtain

$$\sum_{i=1}^{n}\frac{1}{\sqrt{d_i}} = \frac{1}{\sqrt{d_1}}+\frac{1}{\sqrt{d_2}}+\cdots+\frac{1}{\sqrt{d_n}} \ge \frac{n}{\sqrt{\frac{1}{n}\sum_{i=1}^{n}d_i}} = \frac{n}{\sqrt{\frac{2m}{n}}} = \frac{n^{\frac{3}{2}}}{\sqrt{2m}}. \tag{32}$$

By applying the bound of Proposition 16 for regular graphs together with inequality (32), we obtain

$$\mathcal{E}(G) \le \frac{n^2}{\sum_{i=1}^{n}\frac{1}{\sqrt{d_i}}} \le \frac{n^2}{\frac{n^{\frac{3}{2}}}{\sqrt{2m}}} = \sqrt{2mn}.$$

So the upper bound of Proposition 16 for regular graphs is better than the upper bound of Theorem 8.

The next result presents an upper bound for the energy of graphs in terms of order and the general zeroth-order Randić index of graphs.

Theorem 17. *Let G be a graph of order $n \ge 3$ with minimum degree $\delta \ge 1$. Then, for any real number $\beta < 0$ or $\beta > 1$,*

$$\mathcal{E}(G) \le \sqrt[\beta]{(n-1)^{\beta-1}\,{}^0R_{\frac{\beta}{2}}}. \tag{33}$$

Proof. Since, $y > 0$, y^β is a strictly convex function if $\beta < 0$ or $\beta > 1$, we have

$$\left(\sum_{i=1}^{n} \frac{\sqrt{d_i}}{n-1}\right)^{\beta} \leq \sum_{i=1}^{n} \frac{1}{n-1}\left(\sqrt{d_i}\right)^{\beta}.$$

As

$$\left(\sum_{i=1}^{n} \sqrt{d_i}\right)^{\beta} \leq (n-1)^{\beta-1} \sum_{i=1}^{n}\left(\sqrt{d_i}\right)^{\beta},$$

it follows that,

$$\sum_{i=1}^{n} \sqrt{d_i} \leq \sqrt[\beta]{(n-1)^{\beta-1}{}^{0}R_{\frac{\beta}{2}}}. \tag{34}$$

Combining Theorem 9 with inequality (34), we obtain the result. ■

Remark. Setting $\beta = 2$ in Theorem 17, we obtain $\mathcal{E}(G) \leq \sqrt{2(n-1)m}$, which is sharper than McClelland's bound in Theorem 8 for $n \geq 3$, as illustrated in Table 4.

Table 4. Numerical check of Remark: comparison between the bound from Theorem 17 with $\beta = 2$ and McClelland's bound (Theorem 8).

Graph G	n	m	$\mathcal{E}(G)$	Theorem 17 ($\beta = 2$)	Theorem 8
P_{10}	10	9	12.05	12.73	13.42
C_{10}	10	10	12.94	13.42	14.14
$S_{10} = K_{1,9}$	10	9	6.00	12.73	13.42
$K_{4,4}$	8	16	8.00	19.60	16.00
Benzene (C_6)	6	6	8.00	8.49	8.49
Naphthalene	10	11	13.68	14.07	14.83
Anthracene	14	16	19.45	20.40	21.17

The next theorem presents an upper bound on the energy of a graph in terms of its size, order, minimum degree, and maximum degree of a graph.

Theorem 18. *Let G be a graph of order n, size m, maximum degree Δ, and minimum degree $\delta \geq 1$. Then*

$$\mathcal{E}(G) \leq (2m)^{\frac{\sqrt{\Delta}}{\sqrt{\Delta}+\sqrt{\delta}}}\, n^{\frac{\sqrt{\delta}}{\sqrt{\Delta}+\sqrt{\delta}}}. \tag{35}$$

Equality holds if and only if $G \cong \frac{n}{2}K_2$ for n even.

Proof. Using the quadratic and the arithmetic mean inequalities for positive integers $\sqrt{d_1}, \sqrt{d_2}, \ldots, \sqrt{d_n}$, we have

$$\frac{d_1 + d_2 + \cdots + d_n}{\sqrt{d_1} + \sqrt{d_2} + \cdots + \sqrt{d_n}} \geq \frac{\sqrt{d_1} + \sqrt{d_2} + \cdots + \sqrt{d_n}}{n}. \tag{36}$$

Since $\sqrt{d_1}, \sqrt{d_2}, \ldots, \sqrt{d_n}$ are positive integers, it follows that

$$\frac{\sqrt{d_1} + \sqrt{d_2} + \cdots + \sqrt{d_n}}{n} \geq 1 \text{ and } \sqrt{\frac{\Delta}{\delta}} \geq 1.$$

So,

$$\left(\frac{d_1 + d_2 + \cdots + d_n}{\sqrt{d_1} + \sqrt{d_2} + \cdots + \sqrt{d_n}}\right)^{\sqrt{\frac{\Delta}{\delta}}} \geq \left(\frac{d_1 + d_2 + \cdots + d_n}{\sqrt{d_1} + \sqrt{d_2} + \cdots + \sqrt{d_n}}\right)$$
$$\geq \frac{\sqrt{d_1} + \sqrt{d_2} + \cdots + \sqrt{d_n}}{n}.$$

The above inequality yields

$$(2m)^{\sqrt{\frac{\Delta}{\delta}}} \geq \frac{\left(\sqrt{d_1} + \sqrt{d_2} + \cdots + \sqrt{d_n}\right)^{\frac{\sqrt{\Delta}+\sqrt{\delta}}{\sqrt{\delta}}}}{n}. \tag{37}$$

Inequality (37) and Theorem 9 lead to the desired bound.

Suppose that the equality holds in (35). Then all the inequalities in the proof must be equalities. From the equality in (36) we have $d_1 + d_2 + \cdots + d_n = \sqrt{d_1} + \sqrt{d_2} + \cdots + \sqrt{d_n}$ and $\sqrt{d_1} + \sqrt{d_2} + \cdots + \sqrt{d_n} = n$ for $i = 1, 2, \ldots, n$, i.e., $d_1 = d_2 = \ldots d_n = 1$, that is, $G \cong \frac{n}{2}K_2$ for even n. Conversely, if $G \cong \frac{n}{2}K_2$, then it is easy to check that the equality holds in (35). ■

Remark. If G is a regular graph, then $\Delta = \delta$. Hence, applying Theorem 18 for regular graphs, we obtain the same bound as in Theorem 9.

Theorem 19. *Let G be a simple graph of order n with minimum degree at least one. For any non-negative real exponent r, the energy of G is bounded above as follows:*

$$\mathcal{E}(G) \leq \sqrt{\Delta} + \sqrt{\delta} + \sqrt[r+1]{(2m - \Delta - \delta)^r \left({}^0R_{\frac{1-r}{2}}(G) - \Delta^{\frac{1-r}{2}} - \delta^{\frac{1-r}{2}}\right)}.$$

Proof. Consider non-negative real numbers a_i and positive real numbers $\frac{x_i}{a_i}$. Applying Inequality (6) yields:

$$\left(\sum_{i=1}^{n} a_i\right)^r \sum_{i=1}^{n} a_i \left(\frac{x_i}{a_i}\right)^{r+1} \geq \left(\sum_{i=1}^{n} x_i\right)^{r+1},$$

which is equivalent to:

$$\left(\sum_{i=1}^{n} a_i\right)^r \sum_{i=1}^{n} \frac{x_i^{r+1}}{a_i^r} \geq \left(\sum_{i=1}^{n} x_i\right)^{r+1}. \tag{38}$$

Equality in (38) occurs if and only if $r = 0$ or $\frac{a_1}{x_1} = \frac{a_2}{x_2} = \cdots = \frac{a_n}{x_n}$. Substituting $a_i = d_i$ and $x_i = \sqrt{d_i}$ for $i = 2, 3, \ldots, n-1$ into Inequality (38), we obtain:

$$\left(\sum_{i=2}^{n-1} d_i\right)^r \sum_{i=2}^{n-1} d_i^{\frac{1-r}{2}} \geq \left(\sum_{i=2}^{n-1} \sqrt{d_i}\right)^{r+1},$$

which implies:

$$\sum_{i=2}^{n-1} \sqrt{d_i} \leq \sqrt[r+1]{(2m)^r \, {}^0R_{\frac{1-r}{2}}(G)}. \tag{39}$$

The result follows from Theorem 9 and Inequality (39). For even n, equality holds when $G \cong \frac{n}{2}K_2$. ∎

The demonstrations for the subsequent results follow a parallel line of reasoning to that of Theorem 19 and are consequently omitted here for brevity.

Theorem 20. *Consider a graph G on n vertices with minimum degree satisfying $\delta \geq 1$. For any rational parameter $r \geq 0$, the following upper bound on the graph energy holds:*

$$\mathcal{E}(G) \leq \sqrt{\Delta} + \sqrt[r+1]{(2m - \Delta)^r \left({}^0R_{\frac{1-r}{2}}(G) - \Delta^{\frac{1-r}{2}}\right)}.$$

Theorem 21. *Let G be a graph of order n whose minimum degree is at least one. Then, for any non-negative rational value r, the energy is* *bounded by:*

$$\mathcal{E}(G) \leq \sqrt{\delta} + \sqrt[r+1]{(2m-\delta)^r \left({}^0R_{\frac{1-r}{2}}(G) - \delta^{\frac{1-r}{2}}\right)}.$$

Remark. Making $r = 1$ in Theorems 19, 20, and 21, we obtain, respectively, the following inequalities for the energy of a graph G of order n, size m, maximum degree Δ, and minimum degree $\delta \geq 1$:

$$\mathcal{E}(G) \leq \sqrt{\Delta} + \sqrt{\delta} + \sqrt{(2m - \Delta - \delta)(n-2)},$$

which was proved in [11];

$$\mathcal{E}(G) \leq \sqrt{\Delta} + \sqrt{(2m - \Delta)(n-1)},$$

which was proved in [1] and [23]; and

$$\mathcal{E}(G) \leq \sqrt{\delta} + \sqrt{(2m - \delta)(n-1)},$$

which was proved in [32].

We now establish several bounds on graph energy by synthesizing the framework from Remark 2 with established results from Section 2. Setting the parameter $r = 3$ in Remark 2 and invoking Theorem 5 yields the following proposition, which expresses an upper bound for the energy using the graph's order, size, and Narumi-Katayama index.

Proposition 22. *Let G be a graph of order n with minimum degree $\delta \geq 1$. Then,*

$$\mathcal{E}(G) \leq (2m)^{\frac{3}{4}} \sqrt[4]{\left(\frac{2m}{n}\right)^{n-1} \frac{n}{NK(G)}}.$$

Taking $r = 3$ in Remark 2 and applying Theorem 7 leads to the next result, bounding the energy in terms of the graph's size and its atom-bond connectivity index.

Proposition 23. *Let G be a graph of order n with minimum degree $\delta \geq 2$. Then,*

$$\mathcal{E}(G) < (2m)^{\frac{3}{4}} \sqrt[4]{ABC(G)}.$$

Setting $r = 3$ in Remark 2 and employing Theorem 6 provides an energy bound for trees that incorporates order, size, and diameter.

Proposition 24. *Let T be a tree of order $n \geq 3$ with minimum degree $\delta \geq 1$ and diameter $diam(T)$. Then,*

$$\mathcal{E}(T) \leq (2m)^{\frac{3}{4}} \sqrt[4]{\frac{3n}{2} - diam(T)}.$$

Finally, taking $r = 3$ in Remark 2 and using Theorem 4 yields an energy bound for trees that involves order, size, and matching number.

Proposition 25. *Let T be a tree of order $n \geq 2$ with minimum degree $\delta \geq 1$ and matching number $\vartheta(T)$. Then,*

$$\mathcal{E}(T) \leq (2m)^{\frac{3}{4}} \sqrt[4]{\frac{5}{4}n - \frac{1}{2} + \frac{2}{n} - \vartheta(T)}.$$

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