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THE TOTAL π-ELECTRON ENERGY SAGA - CONTINUATION

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ABSTRACT. The total π-electron energy, as calculated within the Hückel molecular orbital approximation, is a much studied quantum chemical characteristics of unsaturated conjugated compounds. Its theory, together with that of its modification called "graph energy", was outlined in a review published in 2017 (GUTMAN and FURTULA, 2017). In the present paper, we present the main features of these theories, with emphasis on what happened after 2017. We also mention a few data that are not found in the mentioned review.

Keywords: total π-electron energy, graph energy, Hückel molecular orbital theory

GENESIS

Erich Hückel (1896-1980) is a German physicist, one of the pioneers of quantum chemistry. In the 1920s, working with Peter Debye, he developed a revolutionary theory of strong electrolytes, nowadays known as the Debye-Hückel theory. In the 1930s, in order to get a physics professor position at the Marburg University, he was required to present a new habilitation thesis in the field of physics. He decided to apply quantum theory to some chemical problem. Erich's brother Walter was an organic chemist, and he suggested to Erich to try to resolve the century-old "Benzolproblem". To do this, Erich elaborated an approximative approach towards the solution of the Schrödinger equation pertaining to the π-electrons of benzene. The paper (HÜCKEL, 1931) is just the first in a long series of Hückel's publications in this field, and provides the basis of what nowadays is called Hückel molecular orbital (HMO) theory.

The initial success of the HMO theory was remarkable. According to it, the six π-electrons of benzene form a closed-shell system. The same happens with 4n+2 circularly arranged π-electrons (as in cyclopentadienyl anion, cyclopropenyl cation, …) in stark contrast to 4n circularly arranged π-electrons (as in cycloplentadieny cation, cyclobutadiene, cyclopropenyl anion, …), that form an open-shell system. In addition, the total π-electron energy of benzene is $6\alpha+8\beta$, whereas the π-electron energy of three isolated double bonds is $3(2\alpha+2\beta) = 6\alpha+6\beta$. The energy difference, equal to 2β, would be the stabilization caused by

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cyclic delocalization of the π-electrons in benzene, resulting in its outstanding chemical stability. The predictions of HMO theory with regards to other monocyclic polyenes was eventually found to be in excellent agreement with experimental facts, but only for those species that have a planar geometry (*e.g*., violation occurs in the case of cyclooctatetraene).

It was found that HMO theory can be applied also to other conjugated π-electron systems, both acyclic and polycyclic, both hydrocarbons and heteroatom-containing (COULSON *et al.,* 1978; KUTZELNIGG, 2007). HMO theory gained much of its popularity after the publication of the book (STREITWIESER, 1961), in which numerous correlations between experimentally determined values and those calculated by HMO were presented. The chemical applicability of the HMO model was especially convincing in the case of benzenoid hydrocarbons, and especially in the case of their total π-electron energies (GUTMAN and POLANSKY, 1986; GUTMAN, 1992).

After the appearance of more powerful computers, and more accurate quantum-chemical methods, HMO theory gradually lost its importance. Nowadays it is used solely for teaching purposes.

However, the HMO total π-electron energy survived, and is nowadays a much studied mathematical object with surprisingly many applications. This will be fully documented in what follows and is the main message of this paper.

BASIC FACTS ON HMO TOTAL π-ELECTRON ENERGY

The molecular orbitals in HMO theory are formally assumed to be a linear combination of the wave functions of p-electrons, each located on a particular carbon atom (or heteroatom). Let the number of such basis functions be n (in the case of benzene: n = 6). Then the respective Hamiltonian operator $\boldsymbol{H}$ is a square matrix of order n. For conjugated hydrocarbons, the elements of this matrix are given by

$H_{ii} = \alpha$ for all $i = 1,2,\ldots,n$,

$H_{ij} = \beta$ whenever there is a sigma covalent bond between the i-th and j-th atoms,

$H_{ij} = 0$ whenever the i-th and j-th atoms are not covalently bonded.

The parameter α is called Coulomb integral; in most applications its actual value is irrelevant. The parameter β is referred to as the resonance integral; it is important that its value is negative. In the case of heteroatom-containing conjugated molecules, the parameterization of $\boldsymbol{H}$ is somewhat more complicated, see (STREITWIESER, 1961).

According to the above definition, in HMO theory the matrix $\boldsymbol{H}$ can be written as

$$\boldsymbol{H} = \alpha \boldsymbol{I} + \beta \boldsymbol{A}$$

where $\boldsymbol{I}$ is the unit matrix of order n, whereas $\boldsymbol{A}$ is a symmetric (0,1)-matrix that can be interpreted as the adjacency matrix of a graph, namely of the molecular graph of the underlying conjugated molecule; for details see (GUTMAN and POLANSKY, 1986). Recall that

$A_{ii} = 0$ for all $i = 1,2,\ldots,n$,

$A_{ij} = 1$ whenever there is an edge between the i-th and j-th vertices,

$A_{ij} = 0$ whenever the i-th and j-th vertices are not connected by an edge.

Then the molecular orbital energy levels are equal to

$$E_i = \alpha + \beta \lambda_i \ , \ i = 1,2,\ldots,n \tag{1}$$

where λ_i, $i = 1,2,\ldots,n$, are the eigenvalues of the adjacency matrix, forming the spectrum of the molecular graph. For details of the theory of graph spectra see, for instance, (CVETKOVIĆ *et al.,* 2010).

This connection between HMO and spectral graph theory was formally recognized in 1956 (GÜNTHARD and PRIMAS, 1956) but was certainly known earlier. Surprisingly, the first mathematical paper on spectral graph theory appeared a year later (COLLATZ and SINOGOWITZ, 1957).

It can be conjectured that Collatz and Sinogowitz, and possibly other scholars, read Hückel's papers from 1930s, and recognized their graph-theoretical mathematical connection. The time gap between Hückel's molecular orbital model (in the 1930s) and graph spectral theory (in the late 1950s) may be explained by World War II and the destruction that happened in Germany during and after it. Anyway, extensive application of spectral graph theory in HMO theory started in the 1970s and is ongoing ever since; see (GUTMAN and FURTULA, 2017) and the references quoted therein.

Using Eq. (1), the total energy of the π-electrons is

$$E_\pi = \sum_{i=1}^{n} g_i\, E_i = \sum_{i=1}^{n} g_i [\alpha + \beta \lambda_i]$$

where g_i is the occupation number of the *i*-th molecular orbital. Usually, if *n* is even ($n = 2k$), then

$$g_1 = g_2 = \cdots = g_k = 2 \ , \ g_{k+1} = g_{k+2} = \cdots = g_n = 0$$

whereas if *n* is odd ($n = 2k+1$), then

$$g_1 = g_2 = \cdots = g_k = 2 \ , \ g_{k+1} = 1 \ , \ g_{k+2} = g_{k+3} = \cdots = g_n = 0$$

which results in

$$E_\pi = \begin{cases} n\,\alpha + \beta \left[2 \sum_{i=1}^{n/2} \lambda_i \right] & \text{if } n \text{ is even} \\ n\alpha + \beta \left[\lambda_{(n+1)/2} + 2 \sum_{i=1}^{(n-1)/2} \lambda_i \right] & \text{if } n \text{ is odd} \end{cases} \tag{2a}$$

or, using the standard β-units:

$$E_\pi = \begin{cases} 2 \sum_{i=1}^{n/2} \lambda_i & \text{if } n \text{ is even} \\ \lambda_{(n+1)/2} + 2 \sum_{i=1}^{(n-1)/2} \lambda_i & \text{if } n \text{ is odd} \end{cases} \tag{2b}$$

GRAPH ENERGY

Formulas (2a) and (2b) have an important special case. Namely, for a large class of molecular graphs (including those of benzenoid hydrocarbons and acyclic polyenes), the relation (3)

$$E_\pi = n\alpha + \beta\sum_{i=1}^{n}|\lambda_i| \qquad \text{i. e.,} \qquad E_\pi = \sum_{i=1}^{n}|\lambda_i| \tag{3}$$

holds; details can be found in (GUTMAN and POLANSKY, 1986; GUTMAN and FURTULA, 2017) and elsewhere. Formula (3) holds for conjugated π-electron systems in which all bonding MO energy levels are doubly occupied, and all antibonding MO energy levels are empty.

The special case (3) was known to many early authors, in particular to Charles Coulson and Bernard McClelland (COULSON, 1940; MCCLELLAND, 1971).

Formula (2a) and its simplified version (2b) are so awkward and complicated that it is not to be expected that mathematically oriented scholars will be willing to spend their time and attention to their investigation. On the other hand, formula (3), especially its right-hand side, could be expected to be sufficiently attractive to mathematicians. This expectation motivated the present author to define the energy of a graph *G* (of any graph) as

$$E = E(G) = \sum_{i=1}^{n}|\lambda_i| \tag{4}$$

where n is the number of vertices of *G*, and $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of the graph *G*, *i.e.*, the eigenvalues of the adjacency matrix of the graph *G*. This definition was published in 1976 in an insignificant journal (GUTMAN, 1978), which later became a citation classic.

As will be seen below, this chemically motivated graph-spectral concept had a great impact on the development of the studies of the HMO total π-electron energy and, equally, on research in spectral graph theory. Therefore, the following should be made clear:

1) **In the time of publication of the paper (GUTMAN, 1978), its author was Assistant Professor at the Faculty of Science of the University of Kragujevac.**
2) **Therefore, the concept of graph energy should be (in fact: must be) considered as a result obtained at the Faculty of Science and at the University of Kragujevac.**
3) **So far, the concept of graph energy is the greatest (or, at least: one of the greatest) scientific achievements of people working at the University of Kragujevac, including its Faculty of Science.**
4) **Graph energy belongs among the most influential and world-wide accepted scientific concepts created in Serbia, in the second half of the 20th century.**
5) **In the time of writing of the present paper, the members of the scientific community of Serbia, including the people at the University of Kragujevac and its Faculty of Science, are not prepared to accept the claims 1)-4) and to act accordingly. It may be that a time comes when they will be.**

In what follows, a few data will be presented, justifying claims 3) and 4). More can be found in (GUTMAN and FURTULA, 2017) and in the books (GUTMAN, 2017; GUTMAN and FURTULA, 2019).

GRAPH ENERGY – CHEMICAL BACKGROUND

In the time when the concept of graph energy was put forward, several results in the theory of HMO total π-electron energy were known. Of these, we mention here the Coulson integral formula (COULSON, 1940)

$$E_\pi = \frac{1}{\pi} \int_{-\infty}^{\infty} \left[n - \frac{ix\phi'(G,ix)}{\phi(G,ix)} \right] dx$$

and the McClelland upper bound (McClelland, 1971)

$$E_\pi \leq \sqrt{2mn}$$

together with McClelland's approximation

$$E_\pi \approx a\sqrt{2mn} \ \ ; \ \ a \approx 0.9 \, .$$

In these formulas, the conjugated molecule considered is assumed to possess *n* carbon atoms and *m* carbon-carbon bonds (*i.e.*, the respective molecular graph *G* possesses *n* vertices and *m* edges). $\phi(G,\lambda)$ denotes the characteristic polynomial of the molecular graph, $\phi'(G,\lambda)$ is its first derivative, and $i = \sqrt{-1}$. All these results hold if and only if the total π-electron energy satisfies the condition (3). Consequently, the above results would automatically hold also for graph energy.

Thus, at the moment when the concept of graph energy was introduced, several significant mathematical results were known to hold for it (Gutman, 1978). The author hoped that because of the simplicity of the expression (4), some mathematicians will start to study it, thus enhancing the theory of HMO total π-electron energy, thus helping chemists to get a deeper insight into the quantum-theoretical description of conjugated π-electron-containing molecules. This indeed happened, but to an extent that the author did not anticipate.

GRAPH ENERGY – PER ASPERA

In spite of the author's great expectations, after the publication of the paper (Gutman, 1978) nothing happened. Not a single colleague showed any interest in graph energy, not a single paper on this topic (except a few authored or coauthored by I.G.) was published. This appeared to become I.G.'s scientific fiasco.

This lasted for 20 years. In 1999 things started to change, first slowly and then explosively, see Table 1.

GRAPH ENERGY – AD ASTRA

After a twenty-years of silence, in 1999 the first papers produced independently of I.G. were published. Their authors were from China (Li, 1999; Zhang and Li, 1999) and India (Walikar *et al.,* 1999). Of other early researches on graph energy, we mention here those from Canada (Caporossi *et al*., 1999), Germany and Sweden (Koolen and Moulton, 2001), and Columbia (Rada and Tineo, 2003).

In the book (Gutman and Furtula, 2019), all published papers on graph energy were collected (known to the authors in April 2019), together with the names and countries of all involved researchers. These data were mainly generated by internet search. In (Gutman and Ramane, 2020), this census was completed for 2019. After that time no systematic bibliographic research along these lines was done. Therefore, the data displayed in Table 1 for the time after 2019 are certainly and grossly incomplete.

In Table 1 we give the number of papers published in a given year and add some short comments. These numbers slightly differ from those in the book (GUTMAN and FURTULA, 2019), because in the meantime a few more relevant publications were discovered.

Table 1. Published papers on graph energy.

year	papers	comment
1999	6	of these 3 authored or coauthored by I.G.
2000	4	of these 3 coauthored by I.G.
2001	14	of these 7 authored or coauthored by I.G.
2002	3	of these 1 coauthored by I.G.
2003	5	of these 1 coauthored by I.G.
2004	10	
2005	16	
2006	11	
2007	37	
2008	56	more than one per week
2009	72	
2010	69	
2011	63	
2012	65	
2013	68	
2014	82	
2015	116	more than two per week
2016	124	
2017	152	almost three per week
2018	139	
2019	156	three per week
2020	113	no internet search done, yet more than two per week
2021	100	incomplete
2022	85	incomplete
2023	77	incomplete
2024	58	incomplete, yet more than one per week

It may safely be said that in our time, scientific investigations of graph energy are enormous, resulting in well over 2000 publications, and quite a few books. No individual could follow the published production in this area (which nowadays is about 2-3 papers each week). Preparing a complete or nearly complete bibliography is also beyond a person's ability and would require the work of a larger team. Maybe AI could help?

It may safely be said that in our time, scientific investigations of graph energy are done worldwide. Authors all over the world were and are involved in such research. They are from the following countries:

Afghanistan, Argentina, Austria, Australia
Bahrain, Belarus, Belgium, Benin, Bosnia and Herzegovina, Brazil
Canada, Chile, China, Columbia, Croatia, Czech
Denmark
Egypt, Ethiopia
Finland, France
Georgia, Germany, Great Britain, Greece
Hungary

India, Indonesia, Iran, Iraq, Ireland, Israel, Italy
Japan
Kuwait
Lebanon
Malaysia, Malta, Mexico, Morocco
Netherlands, Nigeria, Norway
Oman
Pakistan, Philippines, Poland, Portugal
Ruanda, Rumania, Russia
Saudi Arabia, Serbia, Singapore, Slovakia, Slovenia, Somalia,
South Africa, South Korea, Spain, Sudan, Sweden
Taiwan, Thailand, Turkey
Ukraine, United Arab Emirates, United States of America, Uruguay, Uzbekistan
Venezuela
Yemen

As seen, scholars from almost all continents participate in research of graph energy. To our great dismay, Antarctica is missing from our list. So far.

Most numerous researchers come from China and India, followed by Pakistan and Iran. In Serbia, graph-energy-related studies were done in Belgrade, Kragujevac, Niš, Novi Pazar, Novi Sad, Sombor, and some other smaller places.

We end this section by reminding the reader that the origin of this enormous work is in Kragujevac, at the University of Kragujevac. Not many scientific achievements of this caliber have their origin in Serbia.

THE GRAPH ENERGY DELUGE

The mathematics of the Hückel molecular orbital theory is necessarily based on the adjacency matrix of the underlying molecular graph, cf. Eq. (1). Therefore, also the graph energy was originally defined in terms of the eigenvalues of the adjacency matrix, cf. Eq. (4). It was soon recognized that as far as graph energy is concerned, there is no necessity to use the adjacency matrix*, i.e.*, the eigenvalues of other matrices could also be employed.

The first such modification of graph energy was based on the Laplacian matrix – the "Laplacian energy" (GUTMAN and ZHOU, 2006). The Laplacian matrix $\boldsymbol{L}$ of a graph G with n vertices and m edges is defined via its elements as:

$L_{ii} = d_i$ for $i = 1,2,\ldots,n$,
$L_{ij} = -1$ whenever there is an edge between the i-th and j-th vertices,
$L_{ij} = 0$ whenever the i-th and j-th vertices are not connected by an edge,

where d_i is the degree (= number of first neighbors) of the i-th vertex. Then the Laplacian energy of G is

$$LE = \sum_{i=1}^{n} \left| \frac{2m}{n} - \mu_i \right| \tag{5}$$

where $\mu_1, \mu_2, \ldots, \mu_n$ are the eigenvalues of the Laplacian matrix. Recall that for these eigenvalues the relation $\mu_1 + \mu_2 + \cdots + \mu_n = 2m$ holds.

Soon followed the "distance energy", based on the eigenvalues of the distance matrix (INDULAL *et al.*, 2008). After some time, mathematicians (especially from India) recognized that a graph-energy-like quantity can be defined by using any real and symmetric square matrix, especially those that are somehow related to graphs. This resulted in arbitrarily many "graph energies". Their production was further enhanced after the American mathematician Vladimir Nikiforov showed how such energies can be defined also for non-square matrices (NIKIFOROV, 2007).

The "graph-energy deluge" began. In the book (GUTMAN and FURTULA, 2019), more than 170 different "graph energies" are recorded. In (GUTMAN and RAMANE, 2020), pertaining to the year 2019, additional 13 such "graph energies" were registered. Nowadays, their number may exceed 300, although no census after 2019 was made.

Needless to say that in almost all cases, the new "graph energies" are mathematically trivial and worthless, whereas their applicability in any area of human activity is questionable and unproved. In order to stop the deluge, efforts have been made to elaborate a general theory of graph energies, that would include – as special cases – the results for each particular "graph energy" (GUTMAN, 2012; DAS *et al.*, 2018; LI and YANG, 2024). Nevertheless, at the present moment, there is no sign that the deluge is ceasing.

APPLICATIONS OF GRAPH ENERGY

The obvious application of graph energy is in chemistry, where it coincides with the HMO total π-electron energy for the vast majority of conjugated molecules. The most direct application is for calculating standard enthalpy and other enthalpy-related thermodynamic quantities. Details can be found in (GUTMAN and POLANSKY, 1986; GUTMAN, 1992; GUTMAN and SOLDATOVIĆ, 2001; GUTMAN and FURTULA, 2017) and elsewhere.

What came as a surprise, a very pleasant surprise indeed, was the finding that graph energy has got a large number of other applications, in areas far from organic chemistry. In what follows we list a few of them. The present author did not participate in these applications and, therefore, the interested readers are directed to the references quoted.

Crystalography (YUGE, 2017; YUGE, 2018)
Macromolecules (DHANALAKSHMI *et al.,* 2015; PRAŽNIKAR *et al.*, 2019)
Proteins (WU *et al.*, 2015; DI PAOLA *et al.,* 2016; SUN *et al.*, 2016; YU *et al.*, 2017; XU *et al.,* 2020)
Mechanics (GÜNDÜZ, 2009)
Biology (GIULIANI *et al.*, 2014; GAO *et al.*, 2022; GONG *et al.,* 2022)
Biochemistry (BATHS *et al.,* 2014)
Medicine (BOLANOS and AVIYENTE, 2011; DAIANU *et al.*, 2015; DASGUPTA *et al.,* 2015; NITHIN *et al.*, 2021; BANDYOPADHYAY *et al.*, 2024; OUDJER *et al.,* 2024; NAZ *et al.*, 2025; TANG *et al.,* 2025)
Psychology (SOLOVIEV, 2020; PALUMBO *et al.,* 2024; SUBRAMANI *et al.,* 2025)
Linguistics (VIERLBOECK *et al.,* 2025)
Air Traffic (JIANG *et al.*, 2016)
Satellite Communication (AKRAM and NAZ, 2018)
Process Analysis (MUSULIN, 2014a; MUSULIN, 2014b)
Climate Change (PHILLIPS, 2019)
Pattern Recognition (XIAO *et al.*, 2011; XIAO and HALL, 2018)
Image Analysis (SONG *et al.,* 2010; BAI *et al.*, 2014; POURNAMI and GOVINDAN, 2017; SHI *et al.,* 2025; ZHAO and CAI, 2025)
Satellite Image Classification (MENG and XIAO, 2011; ZHANG *et al.*, 2013)

Face Recognition (ANGADI and HATTURE, 2019)
Complex Systems Design (SINHA and DE WECK, 2013; IANDOLI *et al*., 2018; SINHA and SUH, 2018; EDWARDS *et al*., 2024)
Spacecrafts (PUGLIESE and NILCHIANI, 2017)
Electric automobiles (ATHEEQUE and BASHA, 2024)
Terrorism (QI *et al*., 2013).

It should be noted that in most of these applications, the Laplacian energy is employed; see Eq. (5) for its definition.

For instance, the application described in (QI *et al.,* 2013) assumes that by surveillance of telephone conversations of terrorist suspects, a network (multigraph) is created. Then the change of the Laplacian energy of this network, upon the deletion of a vertex is to be calculated (for each vertex). The greatest such change indicates the expected leader of the terrorist group.

In an analogous manner, Laplacian energy serves to recognize the most important features on an image. In complex systems design (including construction of spacecrafts), the aim is to ensure that the system will continue to function if some of its components fail. By means of Laplacian energy, one pinpoints the most critical components.

CONCLUDING REMARKS

Half a century ago, the present author studied the Hückel molecular orbital theory. Then he proposed a minor modification of the HMO total π-electron energy - the *graph energy.* The sole purpose of the graph energy concept was to make the total π-electron energy more attractive to mathematically trained colleagues. It was hoped that the examination of graph energy will lead to a deeper insight into the structure-dependency of total π-electron energy, thus helping chemist to better understand the properties of conjugated molecules. Nothing more was in mind of the present author when he published his paper (GUTMAN, 1978). What happened later went far beyond of his expectations.

First: Thousands of scholars started to do, and are currently doing, research on graph energy. This most pleasing fact shows that the idea was well chosen and fell on fertile scientific ground. Let's ignore the detail that twenty years was needed until somebody understood the idea.

Second: The other most pleasing fact is that graph energy found applications in areas fully outside of the field of chemistry of unsaturated conjugated compounds, equally outside of any quantum theory. Such phenomena several times occurred in the history of science. Scientific concepts, that initially appear to be purely theoretical and of no practical value, sometimes become useful where nobody could have expected.

Third: The total π-electron energy saga does not end in 2025. He who lives long enough will see what follows.

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