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Graph-Theoretical Insights into Cluster Stability – Analysis of 5–11 Atom Systems –

Rika Sekine[1*], Shogo Hayakawa[1], Sota Taki[1], Moemi Sato[1], Haruki Ikegaya[1], Hiroto Kimura[1], Tomoya Nakata[1], Ayumi Murono[1], Yosuke Kobayashi[1]

[1]Department of Chemistry, Faculty of Science, Shizuoka University, 836 Ohya, Suruga-ku, Shizuoka, 422-8529, Japan

*sekine.rika@shizuoka.ac.jp

Abstract. In this study, we systematically analyzed all isomers of 5–11 atom clusters using a graph-theoretical approach and evaluated their maximum Hückel energy (*HE*) within the Hückel approximation. The maximum *HE* increased with the number of bonds, reached a maximum at an intermediate value, and then decreased again, with the peak located near the average of the minimum and maximum possible edge numbers. This relationship was well reproduced by a simple linear expression. The isomers with maximum *HE* were found to have nearly uniform degree distributions, and classification by graph radius (*Gr*) and maximum degree (*Ma*) revealed that they possess compact and homogeneous structural characteristics. By extrapolating these trends, structural features of maximum-*HE* isomers were predicted for clusters with 12–14 atoms. These results demonstrate the effectiveness of a graph-theoretical description for analyzing cluster stability and provide a foundation for extending the analysis to larger clusters and for comparison with first-principles calculations. In a broader context, this topology-based and computationally efficient framework contributes to computational materials science by offering a sustainable and transferable approach to understanding structure–stability relationships across atomistic systems.

Keywords: Graph theory, hückel energy, cluster stability, computational chemistry, metal clusters, sodium clusters

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1. Introduction

Metal clusters represent a crucial class of finite systems for understanding the transition from individual atoms to the bulk solid state. In particular, small clusters exhibit an enormous number of possible isomers, whose stability and electronic properties are highly size-dependent. Early theoretical efforts by Wang *et al*. [1] employed a Hückel model in combination with graph-theoretical concepts to investigate cluster stability, which led to the establishment of a simplified but insightful framework. Subsequent *ab initio* studies by Solov'yov, Solov'yov, and Greiner [2] provided systematic benchmarks for neutral and singly charged sodium clusters up to 20 atoms, including optimized geometries, binding energies, ionization potentials, and vibrational properties.

Building on these pioneering works, Röthlisberger and Andreoni [3,21] carried out *ab initio* molecular dynamics on sodium clusters with up to 20 atoms, revealing structural and electronic trends at finite temperatures. More recently, Sun *et al*. [4,22] identified a distinctive honeycomb-like motif in Na_{20}, while Kronik *et al*. [5,23] reported accurate polarizabilities for Na clusters up to 20 atoms. Huber *et al*. [6,24] combined photoelectron spectroscopy and density-functional theory to determine the structures of Na_{20}^{-}–Na_{57}^{-}, revealing systematic growth patterns involving double-icosahedral cores and Mackay/anti-Mackay overlayers. Calvo and Spiegelmann [7,25] further demonstrated size-dependent melting behavior in sodium clusters. In parallel, Itoh *et al.* [8,26] investigated Na and Cu clusters, emphasizing the role of *sp*–*d* hybridization in their growth behaviors, and Sanchez *et al*. [9,27] demonstrated that nanoscale gold clusters can exhibit unusual catalytic activity, highlighting the broader relevance of 1-valence metal systems.

More recently, Fisicaro *et al*. [10,28] reported a large-scale density-functional database comprising approximately 44,000 isomers of metallic and semiconducting clusters, and analyzed stability trends using structural and electronic descriptors. These studies collectively advanced the field; however, most have focused on identifying the global minima, while little attention has been paid to extracting general structural features common to the entire isomer ensemble.

Although the Hückel method was one of the earliest molecular-orbital approaches, its algebraic framework based on matrix representation and eigenvalue analysis constitutes the conceptual prototype of all subsequent electronic-structure theories, including modern *ab initio* and density-functional methods. The simplicity and transparency of the Hückel framework continue to provide valuable insights into the fundamental relationship between topology and electronic structure. In fact, recent studies have revisited the Hückel approach from an analytical and parameter-free perspective, demonstrating its continued relevance to contemporary quantum chemistry and materials modeling [11]. In this context, our present work employs a graph-theoretical interpretation of the Hückel framework to systematically analyze cluster structures and stability trends.

In parallel, graph-based representations have become central in modern data-driven materials science. Recent developments in machine learning increasingly describe molecules and crystals as graphs—where atoms are represented as vertices and chemical bonds as edges—to predict physical and chemical properties with high accuracy [12]. Similarly, structural networks have been utilized as descriptors for catalytic and energy materials, highlighting the link between bonding topology and macroscopic functionality [13]. These approaches share the same conceptual lineage with Hückel-type models, in which electronic structure is derived from connectivity information. The present study thus bridges classical graph-theoretical quantum models and current machine-learning-based materials frameworks.

Moreover, graph theory continues to be applied in quantitative analyses of complex inorganic frameworks. For example, Mohankumar *et al*. applied graph-theoretical and QSAR-based molecular descriptors to single-chain diamond silicates, demonstrating how degree- and distance-based topological indices capture both stability and electronic characteristics [14]. While the present work statistically analyzes Hückel energies across all graph isomers, Tsuji provided a complementary interpretation by viewing the coefficients of the lowest occupied molecular orbital (LOMO) as graph-centrality measures and discussing local structural stability of individual metallic clusters [15]. Although different in focus, both studies share the same conceptual basis of understanding electronic properties through graph structures.

In this work, we address this gap by performing a graph-theoretical analysis of all connected simple graphs with 5–11 vertices. For each graph, we computed adjacency-matrix eigenvalues and defined the Hückel energy as the sum of the largest occupied eigenvalues. From these data, we identified the maximum Hückel energies, established empirical relations with the number of edges, and introduced classifications based on graph radius and maximum degree. We further extrapolated these descriptors to clusters with 12–14 atoms and compared our predictions with available *ab initio* results. The outcomes highlight both the potential and limitations of graph-theoretical approaches as complementary tools for understanding cluster stability.

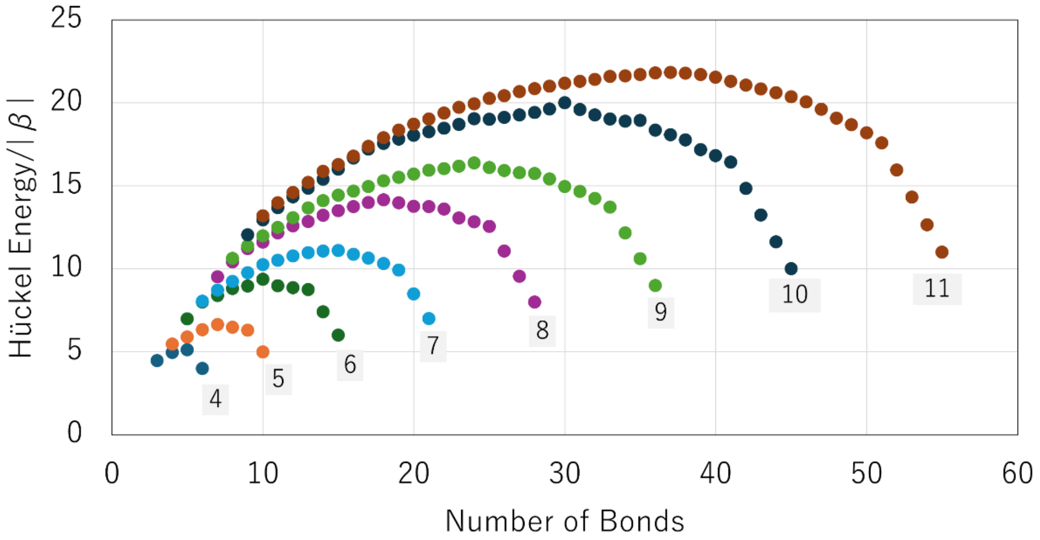


Figure 1. Correlation between maximum Hückel energy and the number of bonds in isomers with 4 to 11 atoms.

2. Methods

2.1. Graph Enumeration

We considered all connected simple graphs with 5–11 vertices, excluding multiple edges and self-loops. The database of isomers used in this work was generated in our laboratory by Taki and is deposited on Zenodo [16]. Equivalent data are also available from McKay's graph database [17]. Our independently generated dataset is consistent with these publicly available resources.

2.2. Adjacency Matrix and Eigenvalues

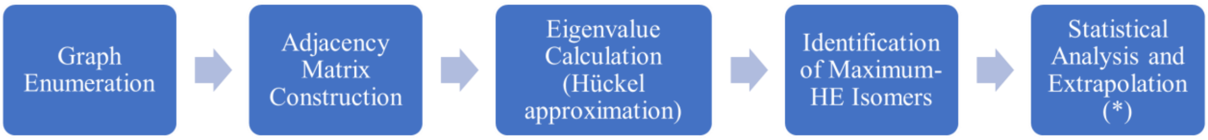
Each graph was transformed into an adjacency matrix A, where the element is 1 if vertices i and j are connected, and 0 otherwise. The diagonal elements were set to 0, making the matrix symmetric. Eigenvalues ε_1, ε_2, …, ε_n were obtained using standard functions in Python (NumPy) and Mathematica.

2.3. Definition and Evaluation of Hückel Energy

The Hückel approximation was chosen for its compatibility with the graph representation, because the Hamiltonian can be directly expressed by the adjacency matrix. For a graph with N vertices, the number of electrons was assumed to be N. Considering spin degeneracy, the floor(N/2) largest eigenvalues were taken as occupied orbitals. The Hückel energy (*HE*) was defined as twice the sum of these occupied orbital eigenvalues:

$$HE = 2\sum_{i=1}^{\lfloor N/2 \rfloor} \varepsilon_i \qquad (1)$$

Using this definition, *HE* values were computed for all graphs for each N, and the structures yielding the maximum *HE* (maximum-*HE* isomers) were identified. Data handling and filtering were carried out using Python (Pandas).



* Linear fit vs. *e_opt*, Classification by *Gr* and *Ma*

Figure 2. Workflow of the graph-theoretical analysis for cluster stability.

Table 1. Relationship between number of bonds and maximum *HE*

Cluster size (*N*)	Minimum number of bonds	Maximum number of bonds	*e_opt*=(Min+Max)/2	Number of bonds for maximum *HE*
5 (pentamer)	4	10	7	7
6 (hexamer)	5	15	10	10
7 (heptamer)	6	21	13.5	15
8 (octamer)	7	28	17.5	18
9 (nonamer)	8	36	22	24
10 (decamer)	9	45	27	30
11 (undecamer)	10	55	32.5	37

2.4. Fitting Procedure

The relation between maximum *HE* and the number of edges was analyzed using polynomial and linear models. The linear form was found to provide the best fit, and fitting was performed with Python numerical libraries (SciPy). The resulting empirical expression was written in terms of the optimal edge number, defined as the average of the minimum and maximum number of edges:

$$e_{opt} = \frac{(N-1) + \frac{N(N-1)}{2}}{2} \qquad (2)$$

2.5. Classification and Extrapolation by Graph Descriptors

For maximum-*HE* isomers, the graph radius (*Gr*) and maximum degree (*Ma*) were calculated using standard graph analysis functions in Mathematica. This allowed us to classify structural features systematically. Based on these descriptors, the empirical relations obtained for 5–11 atoms were extrapolated to clusters with 12–14 atoms to predict the behavior of maximum Hückel energies. Most of the calculations were performed on standard desktop PCs. Only the largest cases, where the number of isomers became too large, were executed on the supercomputing system at Kyoto University.

3. **Results and Discussion**

3.1. Correlation Between Maximum HE and Number of Edges

For all isomers up to 11 atoms, adjacency matrices were constructed and their eigenvalues were computed to obtain the Hückel energy (*HE*). For each edge number, the isomer giving the maximum *HE* was identified. In every cluster size examined, *HE* increased with the number of edges, reached a maximum, and then decreased again (Figure 1). This behavior was consistently observed for clusters with 4–11 atoms, and the maximum *HE* was typically obtained at edge numbers close to the midpoint between the minimum (*N*–1) and maximum (*N*(*N*–1)/2) possible edges.

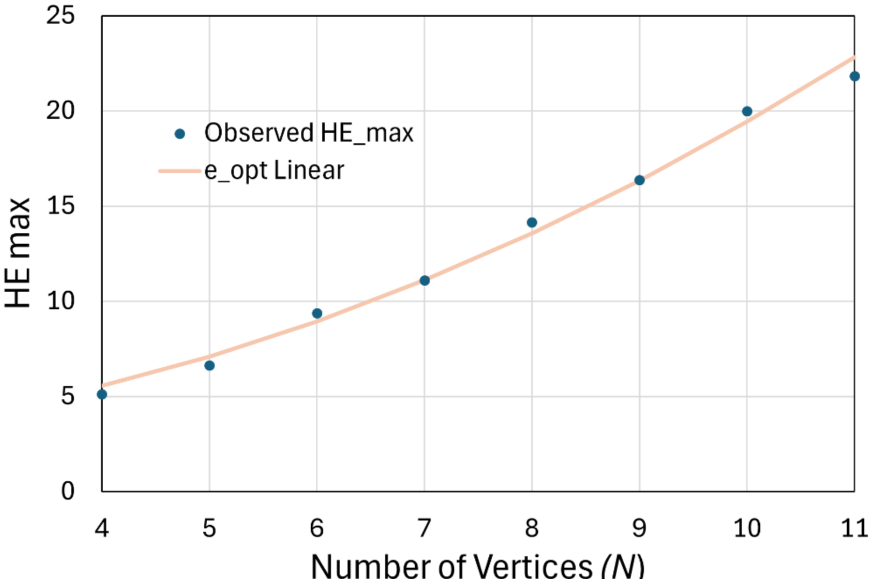


Figure 3. Maximum Hückel energy (HE_max) plotted against the number of vertices (N). Although *HE_max* is not linear in N, it is well reproduced by a linear function of *e_opt*(N), providing a consistent description across $N = 4$–11.

Table 2. Comparison of functional forms for fitting HE_max.

Model	Equation	Coefficients	Remarks
Linear	HE_max = $\alpha \cdot N + \beta$	$\alpha=2.484$, $\beta=-5.520$	Simple, accuracy decreases for large N
Quadratic	HE_max = $\alpha N^2 + \beta N + \gamma$	$\alpha=0.0786$, $\beta=1.3047$, $\gamma=-1.5107$	Fits well overall
Logarithmic	HE_max = $\alpha \log(N)+\beta$	$\alpha=17.016$, $\beta=-20.306$	Accurate for small N, poor for large N
e_opt Linear	HE_max = $\alpha \cdot$ *e_opt* $+ \beta$	$\alpha=0.616$, $\beta=2.787$	High accuracy, easy to interpret physically using *e_opt*
N+1/N	HE_max = $\alpha N+\beta+\gamma/N$	$\alpha=3.045$, $\beta=-13.614$, $\gamma=26.203$	Very high accuracy

This characteristic trend has been reported previously. Sekine *et al.* [18] analyzed sodium clusters up to nine atoms using a graph-theoretical approach and showed that *HE* varies nonlinearly with the number of edges, reaching a maximum near the midpoint value. Similarly, Maeda *et al*. [19] reported consistent results for 5–8 atom clusters, confirming that the maximum *HE* appears near the average of the minimum and maximum edge numbers. In the present study, we extended this analysis to 11 atoms. Specifically, for N = 9, the maximum was observed at 24 edges compared with the midpoint value of 22; for N = 10, at 30 edges compared with 27; and for N = 11, at 37 edges compared with 32.5. These findings reveal a size-dependent trend in which the maximum position gradually shifts to larger edge numbers relative to the midpoint as the cluster size increases (Table 1).

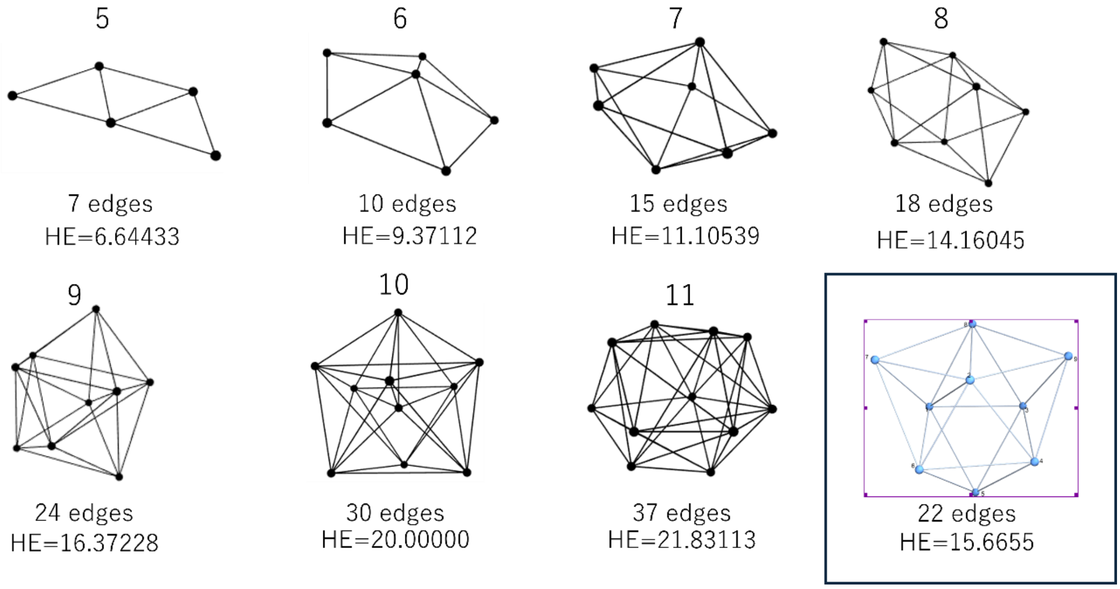


Figure 4. Structures of isomers with maximum Hückel energy. The inset illustrates the 9-atom cluster with 22 edges, identified by our collaborators as the most stable 3D candidate.

3.2. Linear Relationship with e_opt

As shown above, the maximum *HE* is generally obtained at edge numbers close to the average between the minimum and maximum. Based on this, we quantitatively examined the relation between maximum *HE* and *e_opt* for clusters with 5–11 vertices. As shown in Figure 3, a simple linear fit was found to describe the data well:

$$HE\_\mathrm{max} \approx 0.6163 \times e\_opt + 2.7871 \qquad (3)$$

This expression was obtained using Python-based numerical fitting. Reanalysis with Excel gave

$$HE\_\mathrm{max} \approx 0.6132 \times e\_opt + 2.8044 \ \ (R^2 = 0.9915), \qquad (3a)$$

essentially identical results. The coefficients and intercepts agreed up to the second decimal place, confirming that this relation is obtained consistently and does not depend on the analysis method or software environment. A comparison with other functional forms is summarized in Table 2.

This result indicates that cluster stability reaches a maximum at an intermediate bond density. Because each atom has a finite valence, the number of available bonding electrons does not increase proportionally with the number of bonds. As a result, the bond energy per connection gradually decreases as bonding becomes denser, and unlimited stabilization cannot occur. The present analysis revealed that this optimal bonding condition appears near the average between the minimum and maximum possible edge numbers. Furthermore, for clusters up to nine atoms, detailed analysis of vertex degree distributions revealed that the graphs with the highest Hückel energies tend to exhibit small variations in vertex degree; in other words, all vertices share nearly equivalent bonding environments. This trend was also observed in the previous study on sodium cluster isomers [18]. Although the analysis for larger clusters (ten atoms and above) is still preliminary, similar tendencies have been found, indicating that graphs with more uniform connectivity generally yield higher *HE* values.

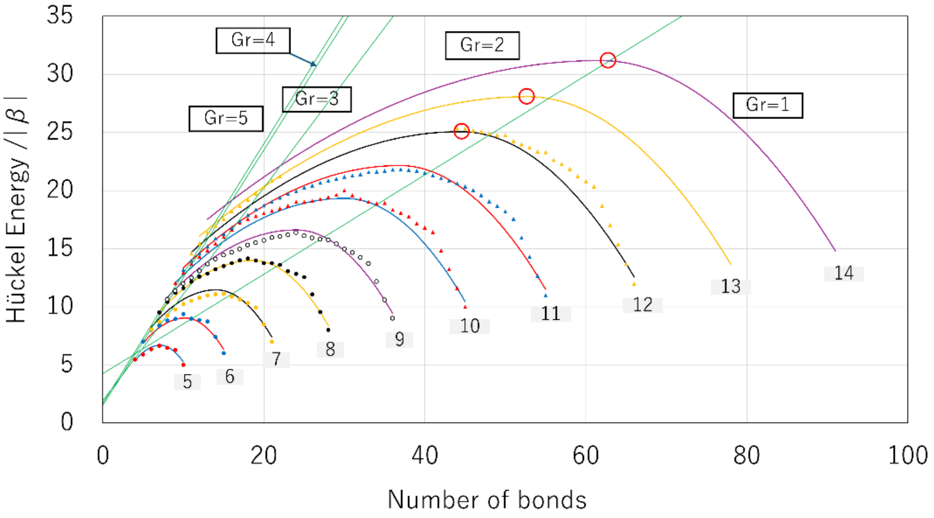


Figure 5. Maximum Hückel energy (*HE*) as a function of the number of bonds (5–14 atoms). The data for $N = 5$–11 are fitted by a parabolic function of edge number, and extrapolations to $N= 12$–14 are also shown. Classification by graph radius (*Gr*) is indicated. The extrapolated maxima for $N = 12$, 13, and 14 are marked with red circles, demonstrating that these points lie in the region of $Gr \approx 2$, consistent with the trend that maximum-*HE* isomers become increasingly compact as the cluster size increases.

Quadratic and $N+1/N$ models achieve higher accuracy, but their expressions are more complex and difficult to interpret physically. In contrast, the linear expression based on *e_opt* maintains sufficiently high accuracy ($R^2 > 0.99$) while allowing an intuitive understanding of cluster stability, and was therefore judged to be the most useful. These results demonstrate that the relationship between maximum *HE* and the number of edges can be adequately described by a simple linear expression, which serves as an effective indicator of the general scaling rule of stability with increasing cluster size.

3.3. Examples of Maximum-HE Isomers

The structures of maximum-*HE* isomers for each cluster size were investigated. As shown in Figure 4, the isomers giving maximum *HE* were extracted for each cluster size. For small clusters, where each vertex has only a few connections, the maximum-*HE* structures tend to be relatively planar. As the number of vertices increases, the degree of each vertex becomes larger, and the structures become more compact and approach spherical shapes.

For clusters up to $N= 8$, the maximum-*HE* isomers coincide with the most stable structures obtained from *ab initio* calculations [2]. For $N \geq 9$, however, graph-theoretical maximum-*HE* isomers are not necessarily realizable as stable three-dimensional structures. For example, collaborative studies in our group indicated that a 9-atom cluster with 22 edges is the most stable candidate in 3D space [20]. This illustrates that graph-theoretical *HE* analysis alone cannot always identify the true global minima and must be complemented by structural feasibility checks. Nevertheless, analyzing isomers in terms of *HE* is not only useful for discussing their stability but also meaningful for classifying their structures from a graph-theoretical perspective.

3.4. Parabolic Fitting and Classification by Graph Descriptor

Up to this point, the maximum Hückel energy (*HE*) has been discussed as a function of the number of vertices N. We next analyzed *HE* as a function of both N and the number of edges e. For $N = 5$–11, the data are well reproduced by a parabolic function:

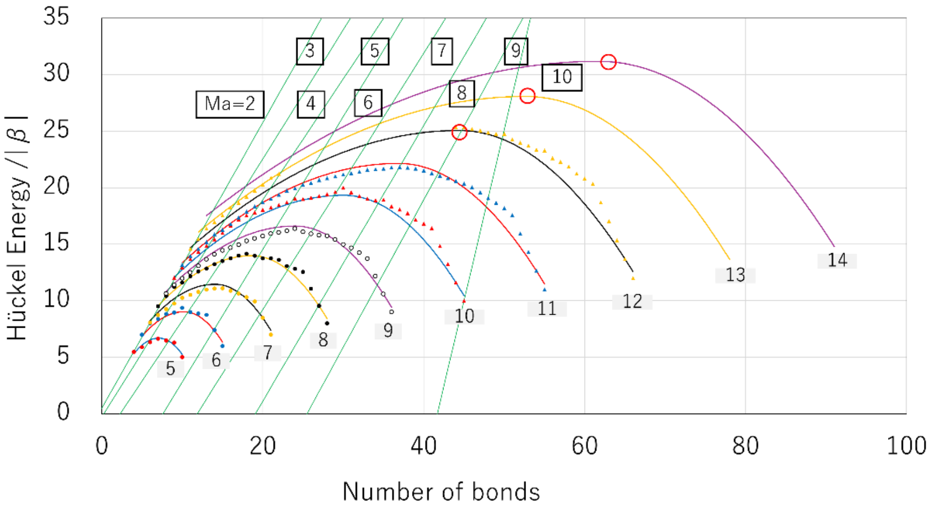


Figure 6. Maximum Hückel energy (*HE*) as a function of the number of bonds (5–14 atoms). The data for *N* = 5–11 are fitted by a parabolic function of edge number, and extrapolations to *N* = 12–14 are also shown. Classification is given by the maximum coordination number (*Ma*) rather than the graph radius (*Gr*). The extrapolated maxima for *N* = 12, 13, and 14 are marked with red circles. These points suggest *Ma* ≈ 8 or 9 for *N* = 12 and *Ma* ≈ 10 for *N* = 13, while for *N* = 14 the maximum-*HE* isomer likely requires *Ma* ≥ 11, indicating the need for further analysis.

$$HE(e, N) = a_N(e - b_N)^2 + c_N$$

$$a_N = -20.846562 \times \frac{1}{N^{3.105506}} \qquad e \leq b_N$$

$$a_N = \frac{0.058887}{N} - \frac{4.576035}{N^2} \qquad e > b_N \tag{4}$$

$$b_N = 0.369048N^2 - 0.940476N + 2.571429$$

$$c_N = 0.048326N^2 + 1.803457N - 3.537159$$

where b_N gives the edge number at the maximum and c_N is the corresponding maximum *HE*. Parameters a_N, b_N, and c_N vary systematically with *N*. Extrapolation of these parameters provides predictions for *N* = 12–14 clusters, as shown in Figure 5. Using the expression for b_N given above (Equation (4)), the predicted edge numbers are ~44, 53, and 62 for *N* = 12, 13, and 14, respectively. These extrapolated maxima are marked with red circles in Figures 5.

Although the analysis for the 12-atom cluster is still in progress, the obtained parameters already confirm that the fitting is valid in both the few-bond and many-bond regions. Furthermore, this extrapolation allows us to predict the overall shape of the curves for the 13- and 14-atom clusters. Classification by graph radius (*Gr*) (Figure 5) revealed that maximum-*HE* isomers consistently had small *Gr* values that converge to 2 as *N* increases. Importantly, the extrapolated points for *N* = 12, 13, and 14—shown as red circles in Figure 5—are located in the region of *Gr* ≈ 2. This trend agrees with the recent large-scale first-principles study by Fisicaro *et al*. [10], which reported that stable isomers generally adopt compact, nearly spherical shapes with small surface area. In graph-theoretical terms, small *Gr* values correspond to short average distances between vertices, supporting this consistency.

Classification by maximum degree (*Ma*) (Figure 6) further revealed that maximum-*HE* isomers align along nearly parallel boundary lines up to $N = 11$. The extrapolated maxima for $N = 12$, 13, and 14 are indicated by red circles in Figure 6. Based on this trend, the most plausible maximum degrees are $Ma \approx 8$ or 9 for $N = 12$ and $Ma \approx 10$ for $N = 13$. For $N = 14$, however, the maximum-*HE* isomer is expected to require $Ma \geq 11$, and further analysis is necessary to clarify this case.

As shown above, for $N = 12$, 13, and 14 the edge numbers giving the maximum *HE* are 44, 53, and 62, respectively. The corresponding total degree sums (2e) are 89, 105, and 123. Assuming that one vertex has $Ma = 9$, 10, and 12 for these clusters, the average degrees of the remaining vertices are approximately 7.2, 8.0, and 8.6, respectively. This suggests that the high degree is not concentrated on a single vertex, but rather distributed almost evenly among the others. In structural terms, the bonding is spread uniformly throughout the cluster, with some variation, but without any single vertex being dominant. As already shown for the maximum-*HE* isomers of 5–11 atom clusters in Figure 4, the variance of degree distribution becomes small for $N \geq 7$, and this trend is expected to persist for $N \geq 12$ as well.

4. Conclusions

In this study, we systematically analyzed all isomers of 5–11 atom clusters using a graph-theoretical approach within the Hückel approximation. The maximum *HE* was found to increase with edge number, reach a maximum near the midpoint between minimum and maximum, and then decrease. This behavior is well described by a simple linear function of *e_opt*. Structural analysis revealed that maximum-*HE* isomers exhibit compact and homogeneous features with small variation in degree distribution. Classification by graph radius (*Gr*) showed a consistent trend toward $Gr \rightarrow 2$ as n increases, while classification by maximum degree (*Ma*) suggested extrapolatable regularities, predicting $Ma \approx 9–11$ (or higher) for $N = 12–14$. Combining parabolic fitting with *Gr* and *Ma* classification thus enables structural predictions beyond 11 atoms. This graph-theoretical framework provides valuable guidelines for assessing stability trends and for comparison with first-principles calculations. Because it relies solely on topological information and simple quantum-chemical approximations, the approach offers a computationally efficient and transferable tool for exploring structure–stability relationships in atomic and molecular systems. Such graph-based descriptors can complement existing first-principles and machine-learning methods in computational materials science, contributing to the sustainable discovery and design of novel materials.

Acknowledgments

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