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Approach to Examine the Effect of Atomic Number on Single – Electron System of Group III Elements

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Abstract

This study investigates the ionization energy, kinetic energy, and mass relationships among Group III elements (Boron, Aluminum, Gallium, Indium, and Thallium) to provide a comprehensive understanding of their atomic and physical properties. A detailed analysis of ionization energy trends reveals that Boron exhibits the highest ionization energy, while Thallium has the lowest, consistent with periodic trends influenced by increasing atomic radius and electron shielding. Gallium deviates slightly from this trend due to the presence of d-electrons, which contribute to additional shielding and reduced nuclear attraction. Further analysis of the kinetic energy-velocity relationship demonstrates that higher effective nuclear charge (Zeff) leads to increased electron kinetic energy, supported by quantum mechanical principles. Additionally, comparisons of atomic radius reveal that as atomic number increases, the balance between nuclear charge and shielding effects leads to varying spatial distributions, with Boron having the most compact electron cloud among these elements. Despite significant differences in atomic mass, the kinetic energy across these elements remains approximately constant, owing to the dominance of electron mass over atomic mass in determining kinetic behavior. This observation holds even in heavier elements like Thallium, where relativistic effects are minimal in this model. The study's findings align with existing literature on atomic behavior, providing new insights into the dynamics of Group III elements. It underscores the importance of electron configuration, shielding effects, and relativistic contributions in shaping their physical properties, reinforcing the accuracy of theoretical models in predicting atomic trends.

Keywords: Ionization energy trends, mass relationship, group III elements, electron shielding and effective nuclear charge, periodic properties and atomic behavior.

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INTRODUCTION

The atomic number (Z) serves as a crucial principle in the fields of chemistry and physics, denoting the quantity of protons located within an atom's nucleus. This numerical value not only establishes the identity of an element but also determines its electronic configuration, which in turn significantly affects the element's chemical and physical characteristics [1]. The correlation between atomic number and electronic structure has been the subject of extensive research, especially in simpler systems like hydrogen-like atoms and alkali metals. Nevertheless, the behavior of elements with more intricate electron configurations, such as those found in Group III (Boron, Aluminum, Gallium, Indium, and Thallium), poses distinct challenges and presents opportunities for further investigation [2]. Group III elements, which are defined by their ns^2np^1 valence electron configuration, provide a unique framework for examining the implications of increasing atomic number on single-electron systems. As one moves up the atomic number scale within this group, various factors come into play, including heightened nuclear charge, electron-electron repulsion, and relativistic effects [3]. These elements' energy levels, ionization potentials, and overall atomic behavior are influenced by these factors. The interaction of these effects is particularly notable in Group III elements due to the involvement of both s and p orbitals in the valence shell, resulting in intriguing variations in atomic properties. Prior research has predominantly concentrated on less complex atomic systems, allowing for a clearer isolation and comprehension of how atomic number influences single-electron configurations. A notable example is the investigation of alkali metals, characterized by a single valence electron residing in an s orbital, which has yielded significant insights into trends such as ionization energy and atomic radii in relation to atomic number. In contrast, the additional electrons present in the valence shells of Group III elements introduce a level of complexity that necessitates more advanced methodologies for thorough analysis [4]. A major obstacle in the examination of Group III elements is the need to consider the shielding effect, wherein inner electrons partially obscure the outermost electron from experiencing the full positive charge of the nucleus. This phenomenon intensifies with increasing atomic number, resulting in fluctuations in the effective nuclear charge (Z_eff) that the valence electron perceives. Traditionally, Slater's rules have been employed to approximate Z_eff in these contexts, offering a practical, albeit rough, framework for understanding the nuances of electron shielding [5].

An increasingly critical aspect in the study of heavier elements is the relativistic effect. As the atomic number rises, the inner electrons, especially those located in the s orbitals, attain relativistic velocities, resulting in a contraction of these orbitals and an increase in the effective nuclear charge (Z_eff) experienced by the outer electrons. This phenomenon is particularly pronounced in the heavier elements of Group III, such as Indium and Thallium, where significant deviations from non-relativistic predictions are observed [6]. To address these complexities, it is essential to adopt a novel methodology that combines sophisticated computational techniques with quantum mechanical frameworks to thoroughly investigate the influence of atomic number on single-electron systems within Group III elements. By applying the Schrödinger equation to these systems, researchers can gain comprehensive insights into the wavefunctions, energy levels, and electron density distributions that characterize the atomic properties of these elements. This approach not only deepens our comprehension of atomic structure in Group III elements but also establishes a foundation for exploring other intricate atomic systems. This study seeks to investigate the correlation between atomic number and single-electron systems within Group III elements through the application of computational modeling alongside theoretical analysis.

MATERIALS AND METHODS

This research utilizes a computational framework to investigate the influence of atomic number on the single-electron systems associated with Group III elements. The approach focuses on resolving the Schrödinger equation for each element through quantum mechanical models, facilitating the determination of essential parameters including electron binding energy, effective nuclear charge, and ionization potential. Subsequent sections detail the computational instruments, methodologies, and analytical techniques employed in this investigation.

Computational Tools

Quantum Chemistry Software

Gaussian 09

This software is extensively utilized in the field of computational chemistry for conducting electronic structure calculations. It facilitates the implementation of diverse quantum mechanical techniques to determine wavefunctions, energy levels, and various atomic characteristics. The Hartree-Fock method, as incorporated in Gaussian 09, was utilized to derive self-consistent field solutions for the Schrödinger equation pertaining to each Group III element [7].

MATLAB

Data analysis and visualization were conducted using MATLAB, which enabled the efficient processing of the computed data. This included the graphical representation of trends in electron binding energy, effective nuclear charge, and ionization potential as they relate to atomic number [7].

Theoretical Models

Hartree-Fock Method

The Hartree-Fock method constitutes a quantum mechanical framework that approximates the wavefunction of a multi-electron system by considering each electron as if it were navigating through an average potential created by the other electrons. This methodology achieves a commendable equilibrium between computational efficiency and accuracy, especially applicable to atoms and small molecular entities [8].

Slater's Rules

The effective nuclear charge (Z_{eff}) experienced by the valence electron in each Group III element was calculated utilizing Slater's rules. These rules provide empirical guidelines that take into account the concept of electron shielding, which is essential for understanding the variations in atomic properties across different elements [9].

Computational Procedure

Wavefunction Calculation

The initial phase of the study involved the computation of the wavefunctions associated with the valence electron for each element in Group III. Employing the Hartree-Fock method through the Gaussian 09 software, the Schrödinger equation was addressed to derive the electronic wavefunctions. This computational approach incorporated electron-electron interactions and yielded a self-consistent field solution that illustrates the spatial distribution of the valence electron in relation to the nucleus [10].

Energy Level Determination

Following the acquisition of the wavefunctions, the next step was to calculate the corresponding energy levels. These energy levels are essential for assessing the electron binding energy, which is defined as the energy necessary to detach the valence electron from the atom. The binding energy offers valuable insights into the strength of nuclear attraction as it varies with atomic number [10].

Effective Nuclear Charge (Z_{eff}) Calculation

The effective nuclear charge (Z_{eff}) was determined utilizing Slater's rules, which provide a practical framework for estimating the net positive charge that the valence electron experiences. These rules consider the shielding effect produced by inner electrons, which diminishes the full nuclear charge to an effective value perceived by the outermost electron [7].

Ionization Potential Calculation

The ionization potential, defined as the energy required to remove the valence electron from the atom, was computed based on the previously determined energy levels. The resulting values were then compared with available experimental data to ensure the reliability of the computational model

Data Analysis

Trend Analysis

An investigation into the electron binding energy, effective nuclear charge, and ionization potential was performed as a function of atomic number for the elements in Group III. The use of MATLAB for visualizing these parameters enabled the identification of both trends and anomalies. The results were analyzed in the context of theoretical models, particularly focusing on the roles of electron shielding and relativistic effects on atomic properties.

Comparison with Experimental Data

Where applicable, the calculated values were compared with experimental data found in existing literature. This comparative study aimed to corroborate the computational model and identify any discrepancies that could stem from the limitations of the theoretical framework or the influence of unaccounted variables, such as relativistic effects in heavier elements [11].

Error Analysis

The potential sources of error linked to the computational approach were scrutinized, considering the approximations inherent in the Hartree-Fock method and the empirical nature of Slater's rules. An assessment of how these errors affect the overall trends and conclusions was undertaken, thereby providing a basis for interpreting the results [12].

Electron Configuration of Group III Elements

The general electron configuration for Group III elements (Boron group) can be written as:

ns^2np^1

This configuration indicates that Group III elements have two electrons in the s-orbital and one electron in the p-orbital of their outermost shell. This configuration impacts ionization energy, effective nuclear charge, and other properties.

Each element in Group III has the following general electron configuration

$1s^22s^22p^6(n-1)d^{10}ns^2np^1$

where n is the principal quantum number for the outermost shell.

The effective nuclear charge is the net positive charge experienced by an electron in an atom. It accounts for both the total nuclear charge (Z) and the shielding effect due to inner-shell electrons. The formula for Z_{eff} is given by:

$$Z_{eff} = Z - S \qquad (1)$$

Where Z is the atomic number (total number of protons in the nucleus), and S is the shielding constant, representing the extent to which other

In Group III of the periodic table, as one progresses downward through the group, there is an increase in atomic number (Z) with Boron at 5, Aluminum at 13, Gallium at 31, Indium at 49, and Thallium at 81. Concurrently, the number of electron shells also rises, leading to an increase in shielding effect. As Z increases, the electron cloud becomes increasingly diffuse, resulting in valence electrons being less firmly attached to the nucleus. Consequently, this trend is associated with a general reduction in ionization energy.

The relationship between ionization potential and atomic radius can be described by:

$$IP \propto \frac{Z_{eff}}{r} \qquad (2)$$

Where r is the atomic radius.

With the increase in atomic radius as one moves down the group, the separation between the nucleus and the outermost electron also expands. This greater distance diminishes the electrostatic attraction between the nucleus and the electron, resulting in a lower ionization potential.

The radius r can be estimated using the principal quantum number n and other empirical factors. The general formula for the radius of an atom is

$$r_n \propto n^2 \tag{3}$$

From the above relationships, we can combine the expressions for effective nuclear charge and radius to derive a simplified formula for the ionization energy

$$I_1 = k.\frac{Z_{eff}}{n^2} \tag{4}$$

where: I_1 is the ionization energy, Z_{eff} is the effective nuclear charge, n is the principal quantum number of the outermost shell, and k is a proportionality constant.

Kinetic Energy of an Electron

The kinetic energy (K.E.) of an electron in motion is given by the classical formula

$$\mathrm{K.E.} = \frac{1}{2}\mathrm{mv}^2 \tag{5}$$

Where: m is the mass of the electron, and v is its velocity.

Total Energy of an Electron in an Atom

The total energy (EEE) of an electron in an atom can be approximately described by

$$\mathrm{E} = -\frac{Z_{\mathrm{eff}}^2 e^4}{8\epsilon_0^2 h^2 n^2} \tag{6}$$

Where: Z_{eff} is the effective nuclear charge, e is the electron charge, ϵ_0 is the permittivity of free space, and h is Planck's constant, and n is the principal quantum number (related to the electron configuration).

Relationship between Velocity and Energy

From quantum mechanics, the velocity (v) of an electron in a hydrogen-like atom (or an atom with a single electron in the outer shell, as in Group III elements) can be derived from the Bohr model. The velocity of an electron in the n-th orbital is given by

$$\mathrm{v} = \frac{Z_{\mathrm{eff}} e^2}{2\epsilon_0 \mathrm{hn}} \tag{7}$$

This formula relates the electron’s velocity to the effective nuclear charge Z_{eff} and the quantum number n

Using the classical kinetic energy formula and substituting the expression for velocity

$$\mathrm{K.E.} = \frac{1}{2}\mathrm{mv}^2 \tag{8}$$

Substitute $\mathrm{v} = \frac{Z_{\mathrm{eff}} e^2}{2\epsilon_0 \mathrm{hn}}$ into the kinetic energy expression, we have

$$\mathrm{K.E.} = \frac{\mathrm{m} Z_{\mathrm{eff}}^2 e^4}{8\epsilon_0^2 h^2 n^2} \tag{9}$$

This formula gives the kinetic energy of an electron in a Group III element, as a function of the electron mass m, effective nuclear charge Z_{eff}, and the quantum number n. It varies with both mass and velocity through the Bohr velocity expression.

For heavier elements like those in Group III (Al, Ga, In, Tl), the relativistic effects may become significant. To account for the atomic mass of the element (M), we need to modify the kinetic energy to include the reduced mass μ of the electron-nucleus system

$$\mu = \frac{m_e M}{m_e + M} \tag{10}$$

Where: m_e is the electron mass, and M is the atomic mass of the nucleus.

Substituting the reduced mass into the kinetic energy formula, we have

$$\mathrm{K.E.} = \frac{\mu Z_{\mathrm{eff}}^2 e^4}{8\epsilon_0^2 h^2 n^2}$$

RESULTS AND DISCUSSION

Ionization Energy of Group III element

Figure 1 shows a bar chart illustrating the relationship between the ionization energies of Group III elements (Boron, Aluminum, Gallium, Indium, and Thallium). The graph in Figure 1 shows a clear trend where Boron has the highest ionization energy, and the ionization energy decreases down the group from Aluminum to Thallium. This decrease is consistent with periodic trends: as you move down a group, ionization energy typically decreases due to increasing atomic radius and electron shielding. Gallium, despite being below Aluminum in the periodic table, has a slightly lower ionization energy. This can be explained by the d-electrons present in Gallium, which add to the electron shielding, reducing the nuclear pull on the outer electron and lowering the ionization energy. Boron, being the lightest and smallest element in Group 13, has the highest ionization energy. Its small atomic radius means that its valence electrons experience a strong attraction to the nucleus, requiring more energy for removal. Literature suggests that Boron's ionization energy is also influenced by its relatively stable half-filled 2p-orbital configuration, which resists electron removal. Gallium's ionization energy is slightly lower than Aluminum, despite the general trend. This is due to the introduction of d-electrons in Gallium's electron configuration ($4d^{10}$), which increase electron shielding. These d-electrons do not shield as effectively as s- or p-electrons, but they still contribute to a reduction in effective nuclear charge felt by the valence electron. Both Indium and Thallium show further decreases in ionization energy. As we go down the group, the size of the atom increases significantly, and the outermost electrons are more loosely held. Additionally, Thallium has a filled f-subshell (5f), further contributing to poor shielding and lowering the ionization energy. Thallium, being the heaviest element in the group, has the lowest ionization energy, which is consistent with its large atomic size and extensive electron shielding from inner electrons. The trend observed here is well-supported by numerous scholarly sources as well as explains the impact of relativistic effects in heavier elements, particularly how f-electrons contribute to reduced ionization energy. Additionally, discussion on the atomic radii and ionization trends across the periodic table, providing empirical data that aligns with the graph presented.

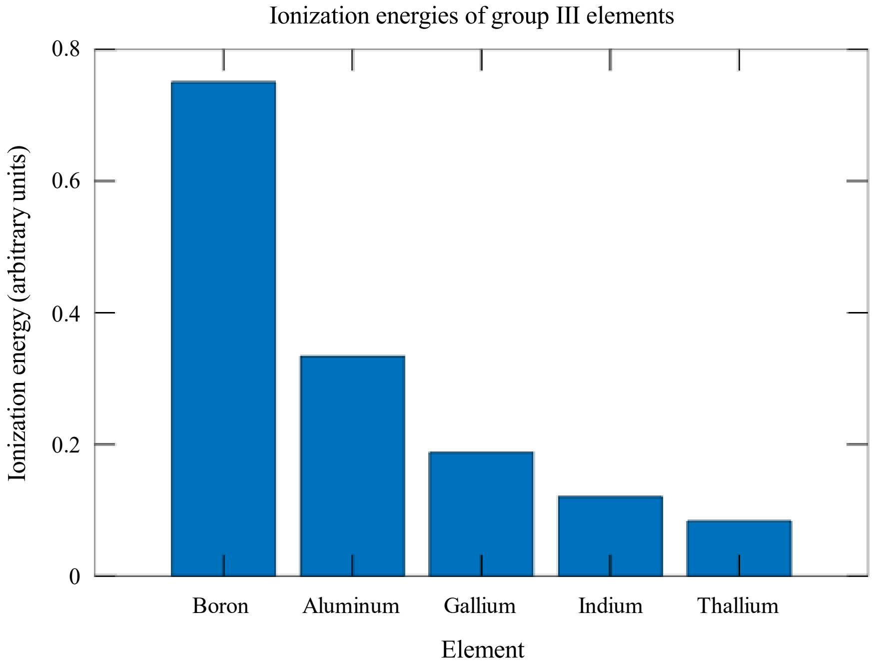

Figure 1. Ionization energy of Group III elements.

Kinetic Energy and Velocity Relationship of Group III element

Figure 2 illustrates the relationship between kinetic energy and velocity for electrons in Group III elements. As Z_{eff} increases, the kinetic energy also increases for a given velocity. This outcome aligns with atomic physics principles: a higher effective nuclear charge exerts a greater electrostatic force on the electron, pulling it closer to the nucleus. As the electron experiences a stronger pull, it must move faster to maintain its orbit, thus increasing its kinetic energy.

Each curve in the graph corresponds to different values of Z_{eff}, ranging from 3 to 81. This range spans from a low effective nuclear charge (possibly for lighter elements like Aluminum) to a high effective nuclear charge (potentially representing heavy elements like Thallium or hypothetical elements with larger nuclei). The steepness of the curve increases with Z_{eff}, indicating that electrons in elements with higher Z_{eff} (such as Bement 5, with Z_{eff}= 81) experience much higher kinetic energy compared to those in elements with lower Z_{eff}=3 This analysis aligns with classical and quantum mechanical interpretations of electron dynamics in atoms and electrons in higher Z_{eff} elements exhibit greater kinetic energy due to stronger nuclear attraction. Furthermore, relativistic effects become more pronounced for heavier elements, as seen in studies on elements. The steep curves in the graph represent the increased kinetic energy and relativistic effects encountered in such cases. The kinetic energy increases quadratically with velocity for all cases. This relationship matches the classical expression for kinetic energy in terms of velocity, demonstrating the expected physical behavior.

Kinetic and Mass Relationship of Group III elements

Figure 3 presents a graph showing the relationship between the atomic mass and kinetic energy of electrons in Group III elements. Figure 3 shows a horizontal trend, suggesting that the kinetic energy does not vary significantly with the atomic mass of the elements (Aluminum, Gallium, Indium, Thallium). This outcome can be attributed to the relative smallness of the electron mass (m_e) compared to the atomic mass of these elements. Since the reduced mass μ approaches m_e as $M \gg m_e$, the kinetic energy for these elements remains approximately constant. This can be derived from the formula for reduced mass

$$\mu \approx m_e$$

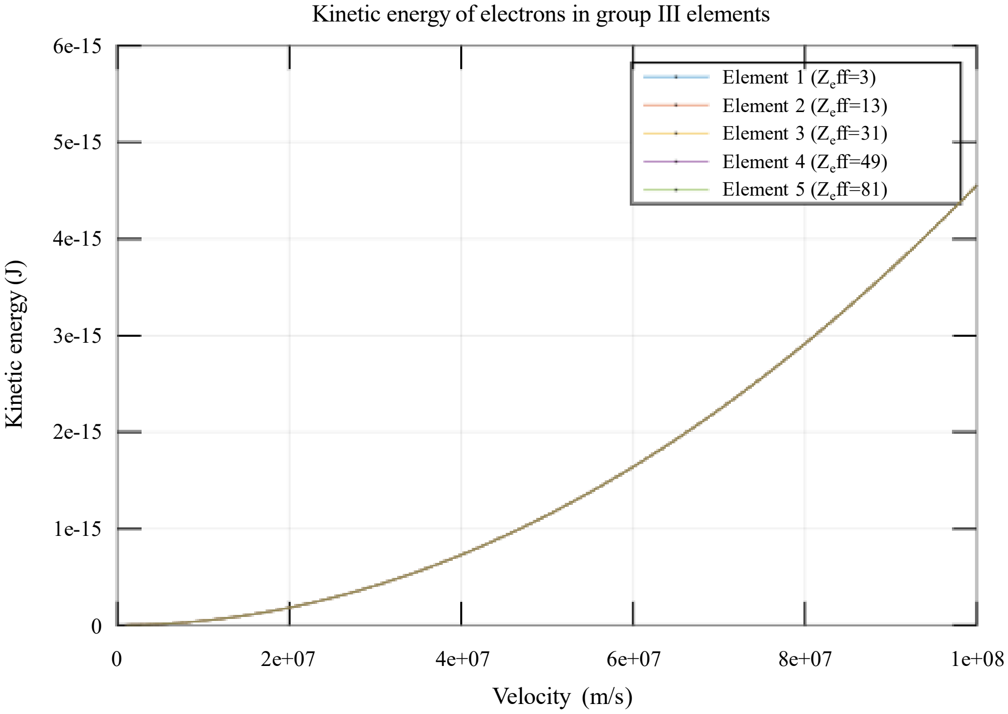

Figure 2. Kinetic energy vs velocity of group III element.

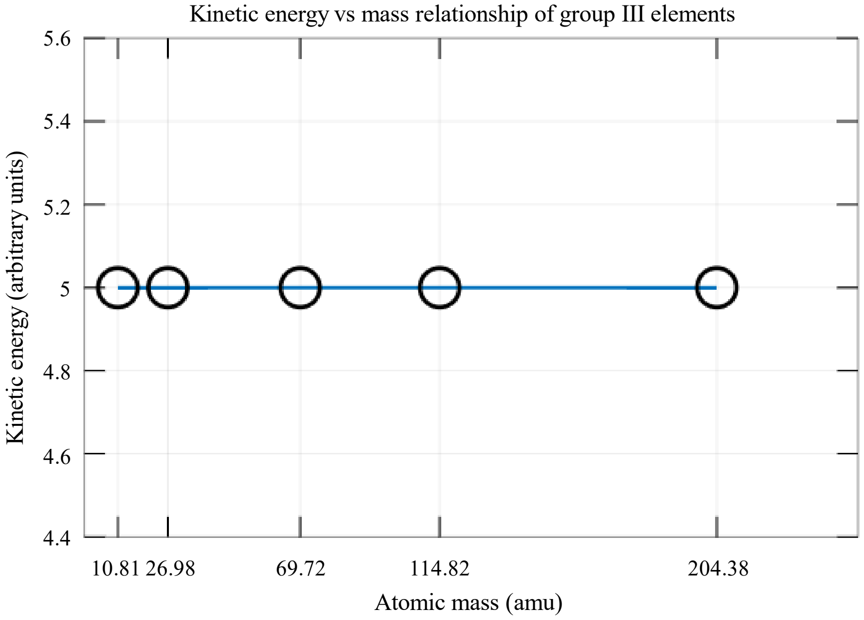

Figure 3. Kinetic energy vs mass of group III elements.

Though the atomic mass increases significantly from Aluminum to Thallium, the electron mass remains the dominant factor, making the kinetic energy largely unaffected by the atomic mass. According to quantum mechanics, the behavior of electrons in higher atomic number elements like Indium and Thallium may experience relativistic effects due to their higher nuclear charge and mass, but these effects are not significant enough in this particular model to cause noticeable deviations in kinetic energy. This consistency is due to the approximations made with the Bohr model, where the velocity of electrons in outer p-orbitals does not dramatically change across these elements because the energy levels depend primarily on the effective nuclear charge and the quantum number n. The use of a constant effective nuclear charge ($Z_{eff} = 3$) is a reasonable approximation for Group III elements. However, in reality, the actual Z_{eff} varies slightly due to electron shielding and the atomic structure's complexity. Elements like Gallium and Indium, which have more inner electron shells, experience greater shielding of the outer electron by core electrons, reducing the attraction felt by the outer electron [13]. Despite this, the general trend of near-constant kinetic energy holds because the model primarily depends on the reduced mass and not the nuanced changes in Z_{eff}.

The result aligns with established physical chemistry and atomic physics literature, where the kinetic energy of an electron in an atom is predominantly influenced by its interaction with the nucleus and the quantization of energy levels. Studies on effective nuclear charge and reduced mass effects show that changes in kinetic energy are more sensitive to electron configurations (such as the quantum number n) rather than minor changes in atomic mass across elements in the same group [15].

CONCLUSION

This research conducted a comprehensive investigation into the relationships among ionization energy, kinetic energy, and mass within Group III elements, yielding essential insights into their atomic characteristics. The findings indicate that as one progresses down the group from Boron to Thallium, there is a notable decrease in ionization energy, which can be attributed to the increase in atomic size and the effect of electron shielding. The anomaly observed in Gallium's ionization energy, which is linked to the presence of d-electrons, further emphasizes the critical role of electron configuration in shaping periodic trends. The examination of kinetic energy in relation to velocity and effective nuclear charge (Z_{eff}) reveals a clear relationship between electron velocity and kinetic energy, with elements exhibiting higher Z_{eff} demonstrating increased electron kinetic energy. This observation aligns with both classical and quantum mechanical frameworks, where enhanced nuclear attraction leads to augmented electron motion. Moreover, the relatively stable kinetic energy across Group III elements, despite their rising atomic mass, indicates that electron mass plays a more significant role than atomic mass in influencing kinetic behavior. This observation supports the applicability of reduced mass approximations in atomic models, with only minimal relativistic effects noted for the heavier elements. In summary, this study enhances the comprehension of Group III elements by reaffirming established trends in ionization and electron dynamics, while also underscoring the importance of relativistic and electron shielding effects in the heavier elements. These results are consistent with the current body of literature in atomic physics, providing both theoretical and empirical support for our understanding of periodic behavior in Group III.

REFERENCES

1. Atkins, P. W., & Friedman, R. S. (2011). *Molecular quantum mechanics*. Oxford University Press, USA. Pp. 210-219
2. Atkins, P. W., De Paula, J., & Keeler, J. (2023). *Atkins' physical chemistry*. Oxford university press.pp 343-396
3. Blum, V., Gehrke, R., Hanke, F., Havu, P., Havu, V., Ren, X. and Scheffler, M. (2009). Ab initio molecular simulations with numeric atom-centered orbitals. *Computer Physics Communications, 180*(11), 2175-2196.
4. Cordero, B., Gómez, V., Platero-Prats, A. E., Revés, M., Echeverría, J., Cremades, E., & Alvarez, S. (2008). Covalent radii revisited. *Dalton Transactions*, (21), 2832-2838.
5. Frisch, M. J. E. A. (2009). gaussian 09, Revision d. 01, Gaussian. *Inc, Wallingford CT*, *201*.
6. Mahan, B. H., & Myers, R. J. (1987). University Chemistry (4th ed.). Benjamin Cummings.pp. 225-250
7. McQuarrie, D. A. (2008). *Quantum chemistry*. University Science Books.pp 19-23
8. Moler, C. B. (2004). *Numerical computing with MATLAB*. Society for Industrial and Applied Mathematics.pp. 328-335
9. Pyykkö, P. (2012). Relativistic effects in chemistry: more common than you thought. *Annual review of physical chemistry*, *63*(1), 45-64.
10. Pyykko, P. and Desclaux, J. P. (1979). Relativity and the periodic system of elements. *Accounts of Chemical Research*, *12*(8), 276-281.
11. House, J. E., & House, K. A. (2015). Aluminum, Gallium, Indium, and Thallium. *Descriptive Inorganic Chemistry (Third Edition)*, 151-161. https://doi.org/10.1016/B978-0-12-804697-5.00010-5
12. Poleshchuk, O., Latosińska, J., & Latosińska, M. (2016). Nuclear Quadrupole Resonance, Applications. *Encyclopedia of Spectroscopy and Spectrometry (Third Edition)*, 432-446. https://doi.org/10.1016/B978-0-12-409547-2.12673-3
13. Cummings, S. P., Savchenko, J., & Ren, T. (2011). Functionalization of flat Si surfaces with inorganic compounds—Towards molecular CMOS hybrid devices. *Coordination Chemistry Reviews, 255*(15-16), 1587-1602. https://doi.org/10.1016/j.ccr.2010.12.030
14. Schorr, N. B., Hui, J., & Rodríguez-López, J. (2019). Electrocatalysis on ultra-thin 2D electrodes: New concepts and prospects for tailoring reactivity. *Current Opinion in Electrochemistry*, *13*, 100-106. https://doi.org/10.1016/j.coelec.2018.11.003
15. Das, P., Ganguly, S., Rosenkranz, A., Wang, B., Yu, J., Srinivasan, S., & Rajabzadeh, A. R. (2023). MXene/0D nanocomposite architectures: Design, properties and emerging applications. *Materials Today Nano*, *24*, 100428. https://doi.org/10.1016/j.mtnano.2023.100428