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Calculate Chemical Properties Molecule through Python Tool

Muhammad Aziz[1,2*], and A.N.Sheikh [2]

[1]Institute of Biochemistry University of Balochistan, Quetta, Pakistan.
[2]Pakistan Chemical Computational Society, Pakistan.
[*]Corresponding Author: Muhammad Aziz. Email: aziz1sh@hotmail.com

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Abstract: Computational chemistry software, developed to calculate the chemical properties of molecules, is known as dry research due to it's depend on theoretical calculations rather than lab experimental data collection. This study leverages such software to estimate chemical properties, which is particularly useful for newly synthesized or modified chemical compounds. Upon successful execution, the computational chemistry software generates a log file. The newly developed software in this study is designed to interface with density functional theory (DFT) software output files. It requires only two inputs from the user i.e the Highest Occupied Molecular Orbital (HOMO) and the Lowest Unoccupied Molecular Orbital (LUMO) values. The software processes the input parameters to generate several key chemical properties, including ionization energy, electron affinity, hardness, chemical potential, electronegativity, softness, and electrophilicity index. Each of these parameters provides valuable insights into the chemical behavior of compounds. The software achieves an acceptable result with a 98.8% confidence interval. Utilizing this third party software is intended to add new features and increase the functionality of current platforms. The tool's emphasis on adaptability, readability, and user-friendliness is consistent with the fundamental ideas of simplicity and adaptability. By offering quick response, this tool HMG.A1 not only closes the gap but also presents opportunities for growth into other computational approaches, advancing studies in areas like materials science, drug discovery, and catalysis.

Keywords: Global Reactivity Descriptors; Python Suit; Chemistry Calculations

1. Introduction

Computational chemistry is an important area of scientific research since it supports the rapid and efficient discovery of new knowledge and solutions to numerous issues in the field of pharmaceuticals, materials science and the conservation of the environment. Its application is not limited to any particular field where educational institutions, industries, and other aspects of society itself gain essential improvement as powerful tools for molecular and material analysis become available to the researchers and engineers. One of the greatest strengths of computational chemistry is the predictive ability of the behavior of molecules or materials depending on their conditions. They will be able to predict molecular structures that will possess certain properties best fit for a particular use, making it a useful tool for material and chemical engineers. Normally, computation chemistry quantum software, which may be rooted on DFT, commonly produces a log file. These 3D conformation can be further viewed with third party molecular graphic tools, which often gives details on the Highest Occupied Molecular Orbital (HOMO) & the Lowest Unoccupied Molecular Orbital (LUMO).Nevertheless, there is an increasing demand for other freeware tools which would allow an analysis

of other properties and calculations based on the DFT log file development of new materials, and environmental protection. Its impact spans various sectors, benefiting educational institutions, industrial applications, and society at large by providing researchers and engineers with powerful tools for molecular and material analysis. A primary advantage of computational chemistry lies in its predictive capabilities regarding molecular or material behavior under varying conditions. This predictive capability facilitates the design of new molecular structures with specific properties tailored for various applications, making it an invaluable resource for material and chemical engineers. Typically, computational chemistry quantum software, often based on Density Functional Theory (DFT), generates a log file after processing. This file can be visualized and interpreted using third-party molecular graphics software, which commonly provides information about the Highest Occupied Molecular Orbital (HOMO) and the Lowest Unoccupied Molecular Orbital (LUMO). However, there is a growing need for additional freeware tools that can further analyze and calculate a range of chemical properties from DFT log file. They should be user friendly so that to minimize the amount of time taken in doing many calculations and to help the work of analysis. Various published researches show that life sciences researchers have weak attitude towards mathematical computations [1], students particularly have difficulty in analyzing graphs and diagrammatical illustrations [2]. Further, there are around thirty millions of color blind people in the whole world and therefore it is obligatory that the new tools are considered with this concern. This consists in checking that software is fully accessible to current accessibility standards, and thus, being able to be used by persons with different degrees of vision deficiency. In conclusion, the creation of available and easy to use recursive freeware, based on DFT data, is fundamental for the progress of computational chemistry. These tools do not only improve the degree of precision and speed of calculations related to chemical properties but also bear strong policy of equality for all users in line with other general goals of scientific discovery and technological development of Quantum chemistry software constitute one of the most specialized sub-genres of computer software or applications aimed in the modeling and prediction of atomic and molecular systems based on quantum mechanics [3]. Such tools are used to determine electronic structure and qualities of molecules [4], estimate chemical processes, and reveal molecular configurations with precision. Computational chemistry, particularly the use of quantum mechanical models such as DFT, has transformed industries like pharmaceuticals, where understanding molecular interactions aids in the prediction of therapeutic efficacy and toxicity. These technologies also aid material research, allowing scientists to create novel materials with improved capabilities for electronics, catalysts, and renewable energy solutions. For example, DFT has been used to anticipate the behavior of materials used in solar cells and batteries, allowing them to be optimized long before experimental testing is performed. Computational chemistry, particularly the use of quantum mechanical models such as DFT, has transformed industries like pharmaceuticals, where understanding molecular interactions aids in the prediction of therapeutic efficacy and toxicity. Furthermore, material science greatly benefits from these technologies. Scientists can create novel materials for electronics, catalysts,

In this pilot study, the molecular behavior computation tool chosen is the open source quantum chemistry software GAMESS (General Atomic and Molecular Electronic Structure System) [5]. In choosing the particular quantum chemistry software there are several determining factors, such as; the research necessities of the particular project, the capacity of the computational class being used and the favorite choice of the chemist. Surprisingly, investigators select programs that are in sync with their research goals and easy to use for computations. To study molecular orbitals therefore including the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO)| a quantum chemistry program that supports molecular orbital calculations is used. The output file provides the information of electronic structure of the molecule involved of HOMO LUMO energies and wave functions based on the results of the above calculations. The energy difference between these orbitals, known as the HOMO-LUMO gap [9], is a focal variable. This gap is used to predict a molecule's reactivity, and its optical characteristics including its electronic absorption, and emission spectra. The method of determining HOMO LUMO gap is by following the procedure of deducting the value of LUMO energy from the HOMO energy. This step may take considerable amount of time, if done

in a manual way. Additional chemical results and analyses need to be obtained and, unfortunately, users need to manually enter the data extracted from the log file.

Despite the rich molecular analysis capabilities of GAMESS and other quantum chemistry applications, saving output data momentarily is quite cumbersome. That is why simplifying this technique and using, for instance, computational tools to tackle these computations may greatly enhance productivity and the time needed to gain chemical insights. HMG.A1 was built with this type of application in mind unlike some of the well-known computational chemistry tools, which can be more time consuming and could cost a user a lot of money acquiring the proper software license or access to a high-performance computing set. This is because the tool's System requirements as well as compatibility with readily available Operating systems like the Microsoft Windows makes it easy for education institutions as well as small research centers who may not make handsome cash or even afford complex systems. Moreover, HMG.A1 can be better understood by students and early career researchers as it has been implemented in Python by the authors.

2. Software Description

The tool known as HMG.A1 is a python program mainly used in computational chemistry, which anyone can download freely. The tool is not demanding when it comes to the system requirements.

Platform and Compatibility, HMG.A1 can be run on any Microsoft window which makes user access easier.

Characteristics of Use The software reported has minimum system requirements that make it compatible with almost any personal computer and even some laptops as it is coded to be resistant to low capacity hardware.

Main Module. The HMG.A1 provided single main module for input value.

This tool's user interface is a single page and makes user interactions easier due to it's simply look. The Lowest Unoccupied Molecular Orbital (LUMO) and Highest Occupied Molecular Orbital (HOMO) energies are represented by two integer values that users manually enter. The tool streamlines the data entry procedure by eliminating the need for a pointer.

HMG.A1 calculates a number of important chemical characteristics. A file that contains text with the computation results is produced. Any common text reader program can be used to read and access this output file, making review and analysis simple.

Extra Features include in tool

Support for Monochromatic Vision. The tool's usability for individuals with color vision impairments is improved by its design, which makes it accessible in settings with monochromatic vision.

A system generated reference number and the current date are shown at the program's top, giving users a special identification number for further necessary action.

2.1. Workflow

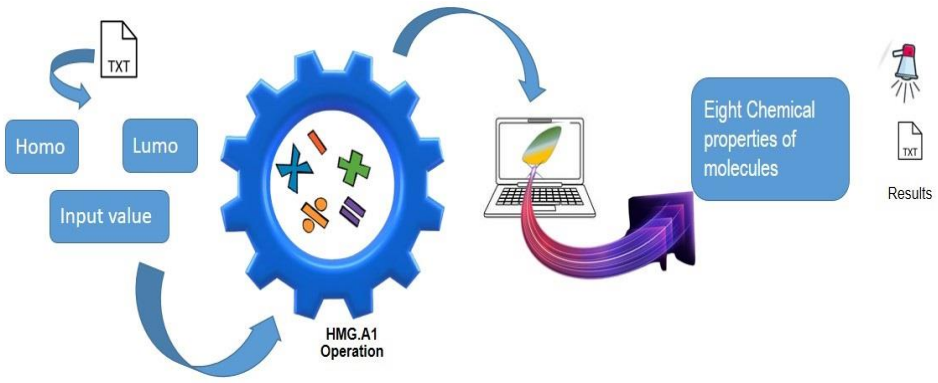

Figure 1. Show a Pictorial Representation of HMG.A1 Tool

You can obtain desired Homo and Lumo values after performing the necessary calculations in quantum chemistry software like Gussian, Gamess, and Pis4. The list is available on the website too. After obtaining the desired value, you can manually enter two integer values.

Within a couple of seconds, six results are prompt ionization energy, electron affinity, hardness [10], chemical potential [11], electronegativity, softness, and electrophilicity index [12].

HMG.A1 generates output in the form of a text file. Which can easily view with any text reader software and display results on a computer screen in monochromatic form, system generated time and ref number is displayed in a text file.

2.2. Security Concern

The development of third party tools necessitates robust security measures to safeguard users from potential risks. Therefore, secure coding methodologies have been implemented in this project to mitigate security risks.

In today's digital research landscape, secure handling of data is essential, particularly when working with proprietary chemical structures or sensitive molecular data. While HMG.A1 is an open source tool, the developers have implemented standardized security measures to ensure that users' computations are protected from potential vulnerabilities. Secure coding methodologies help mitigate risks such as unauthorized data access or software manipulation, ensuring that users can safely rely on the tool for high-accuracy calculations without compromising data integrity.

2.3. Selection Criteria

Currently, one can observe the steady evolution of python in the sphere of chemistry. That is why, python is chosen for the given practical tasks of a chemical informatics nature and for a set of other tasks connected with computational activities in chemistry.

Among them is the work of HMG.A1 automation of computational processes is seen as a major change in how researchers perform chemical analyses. Subsequent releases could incorporate artificial intelligence and machine learning to deliver a far more sophisticated predictive capability than HMG.A1, helping researchers make vastly superior molecular property predictions. Furthermore, the additionally of real time processing for high volume data may provide new possibilities for throughput-based screening and compound optimization. This evolution of the tool aligns with the broader trend toward the use of AI in scientific research, promising to further reduce time, cost, and complexity in computational chemistry.

Given the sensitive nature of some computational chemistry applications, such as proprietary pharmaceutical research or novel material design, the implementation of secure coding practices is critical. Ensuring that the software adheres to rigorous data protection standards is essential to maintaining the confidentiality and integrity of the computational results, particularly when dealing with sensitive or intellectual property data.

2.4. Feature

As seen in figure 2, an automatically produced reference number and date appear at the top of the welcome page. The system returns until the value is entered when the user tries to enter an empty value. The warning value becomes inoperative if you attempt to enter zero. The calculation results are saved in an empty text file that opens after the task is finished.

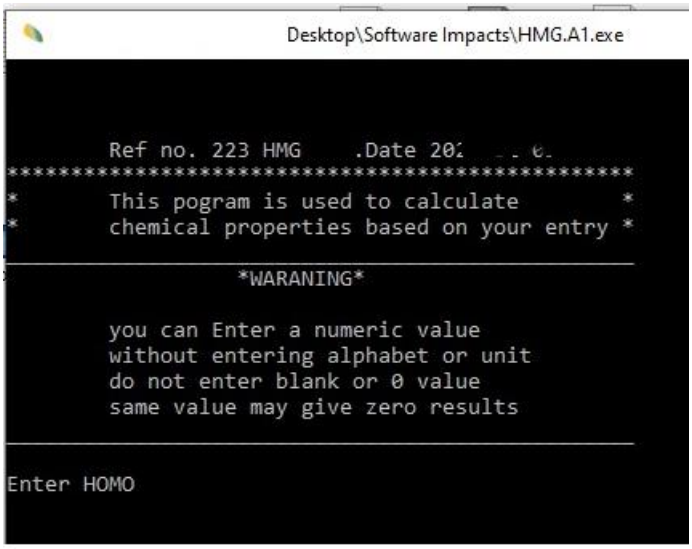

Figure 2. Show main interface of HMG.A1 python tool.

Install the Tool, users can easily download .exe file from Github
https://github.com/aziz1sh1/HMG.A1/blob/main/HMG.A1.exe

3. Helpful Material

The tool HMG.A1 comes with helping material for user.

https://github.com/aziz1sh1/HMG.A1/tree/main

How to use tool (manual.pdf), includes the training manual, instruction manual, and download guide, providing an overview of the tool along with license details.

https://github.com/aziz1sh1/HMG.A1/blob/main/How%20to%20use.pdf

Podcast video include file with contain information how to use tool.

https://github.com/aziz1sh1/HMG.A1/blob/main/method.mp4

Continuously gather feedback from users and stakeholders to iteratively improve HMG.A1 tool. This helps in identifying areas for enhancement and addressing any usability or functionality gaps.

4. Tool Impact

The rapid advancement of computational chemistry and related fields is evident from the extensive body of research available on platforms like Science direct. As of late 2023, a search for research articles on specific key parameters. Such as ionization energy (31,084 articles), electron affinity (46,489 articles), chemical hardness (97,995 articles), and other related parameters reveals over one million articles that incorporate these parameters in their studies. This reflects a significant and growing interest in these areas within the scientific community.

Rapid Development across Computational fields the extensive number of articles and ongoing research indicate that computational fields, including quantum chemistry, are developing rapidly. These fields are not only advancing through new theoretical models and algorithms but are also seeing increased application across various scientific domains. With the expansion of solutions and methodologies, it is expected that standardized practices and widely recognized benchmarks will emerge. These standards will help streamline research and facilitate better comparison and validation of results across different studies. The HMG.A1 Python tool has a significant impact on quantum chemistry research by providing a user-friendly platform for performing essential calculations. It simplifies the process of calculating key chemical properties, thereby improving productivity and efficiency in research activities. The tool aids in streamlining data processing and reducing manual workloads, which is especially valuable in preliminary research phases. Its ability to handle complex calculations and provide clear output makes it an effective preliminary research tool. The user-friendly design of HMG.A1 is crucial for enhancing researcher satisfaction and usability.

A straightforward interface that simplifies data entry and result interpretation contributes to a more efficient research workflow. Effective management and processing of raw data are essential for uncovering hidden chemical properties and gaining deeper insights into molecular systems. Python integrates well with other computational tools and software, allowing researchers to build customized workflows and extend the capabilities of existing systems. Computational methods implemented in Python can estimate chemical properties and predict molecular behaviors much faster than traditional experimental methods.

This rapid computational capability enables researchers to explore various hypotheses, conditions, and scenarios in a relatively short time frame. The ability to quickly test and evaluate multiple conditions accelerates the pace of discovery and development, leading to faster advancements in the field. The HMG.A1 Python tool exemplifies the significant contributions of computational tools to the field of quantum chemistry. By improving productivity, streamlining processes, and enhancing the user experience, it addresses critical needs in computational research. The rapid growth of research in key parameters and the increasing use of Python in computational chemistry underscore the dynamic nature of the field and its potential for continued innovation. As standards evolve and new tools emerge, the integration of advanced computational techniques will further accelerate scientific discovery and development.

HMG.A1 tool help provide quick solutions to some chemical related problems with high precision, and errors are likely to be lesser compared to calculations done manually. This is specifically important in contexts where accuracy and speed in calculation is vital, Convenience HMG.A1 tool are easily install from one computer to other. Making HMG.A1 tool help solve problems and make decisions because they provide numerical answers that help understand data and make decisions on the spot. Consistency HMG.A1 tool use standard procedures of calculation to enhance uniformity of results from one user to the other and from one context to the other. Any age group-user can be used HMG.A1 tool as an aids.

5. Output

After this you will enter a Lumo and Homo value.

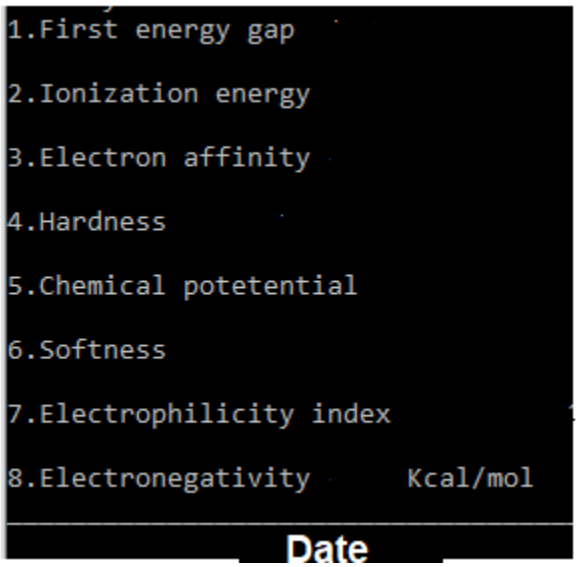

Figure 3. Show output in the form of result, interface of HMG.A1 python tool.

Within couple of seconds following result are generated in screen and prompt finding in text file name result

Figure 4. Automatically create a text file named result.txt.

6. Discussion and Future Works

This type of computer-based calculation tool progresses in a research field known as computational chemistry. The above Python tool provides information in numeric form. There is a need for an upgrade version that allows the end user to visualize the HOMO and LUMO orbitals to understand their spatial distribution and electron density. There is also a need to develop HMG.A1 in an Android app it is always remember a fact; it is difficult to execute computational chemistry tasks on an Android mobile device for a number of reasons including the available processing power and complexity of the calculations to be done, however, performing a full-fledged computational chemistry query on an Android mobile device is not easy but certain options allow at least access to certain facets. However, for serious computational chemistry work, it might be more practical to use other remote computing resources from the android device, or engage in web based interfaces and an online web-based server which provide liberation to run code in web browsers.

Already available tools such as Gaussian, GAMESS, and VASP provide capabilities for molecular simulation, they require significant computational resources, expertise, and few of them are costly licenses, which limit accessibility to smaller research institutions and early career scientists. In contrast, the HMG.A1 tool prioritizes accessibility by reducing system requirements and offering a user friendly interface, making computational chemistry more approachable for a wider audience.

The HMG.A1 tool, which provides the numerical data necessary for assessing molecular characteristics, is a major achievement in the field of computational chemistry. However, there are a number of possible improvements and modifications that might be taken into consideration in order to further improve its usefulness and user experience: now provides a strong framework for doing out necessary molecular orbital computations. It displays output as one or multiple numbers so users can easily determine other important properties like ionization energy, electron affinity, and HOMO-LUMO gap. But as computational chemistry is often related to visual presentation of the structure of a molecule and its electron characteristics there are some demands for this tool which it does not meet. The enhancements designed in the current edition of the HMG.A1 should integrate the ability to display the HOMO and LUMO store. Visualization software enables users to display in a graphical form how orbitals are spatially distributed as well as demonstrating the electron density of each orbital to facilitate learning of molecular activities. This would include the incorporation of graphical representation tools that are capable of displaying 3D orbital plots and electron density maps as well.

There can be some draw back for doing some intensive computational chemistry task on android mobile devices due to their computational capability and the involved calculations even with this it might still be beneficial to develop an Android application version of HMG.A1. Users could observe calculated results, for instance, ionization energy and HOMO LUMO gaps, in their own handset devices. Preview versions of the orbital diagrams could be simplified and appropriate for the mobile devices display. Some of the functions could take advantage of the internet and connect to remote computational facilities or webservers. This would allow users to perform detailed calculations and data visualisations through a web based. To be specific, by using python in web based application development, effective for Python code execution on the web browsers is possible. It meant that users could carry out computational chemistry processes and view them on the web browser interfaces without arising the need to install other applications. Advanced graphical and computational features can be run on the server side but any amount of complexity can be presented to the

user through a browser interface. Enhancing HMG.A1 to also possess better graphical user interface and better graphical capabilities will greatly improve the usability of the software. The execution of such changes would also benefit the low visions users through offering them convenient screens for visualization.

7. Code Explanation

HMG.A1 written in Python script. It performs a chemical calculations which depend on user input and provided the results to both the console and a text file.

I. File Creation and Initialization. A text file named "1.txt" is created using the open () function with write permissions (``w+``), allowing data to be written and read in the same file.

II. Random Number and Date. The code imports the time and date modules to record the current date. The `random` module generates a random integer between 10 and 900, which serves as a unique reference number for the calculation session.

III. Writing Information to File and Console. The initial lines of the program print headers and descriptions both to the console and to the text file. These include caution, how to input values (only numeric values are allowed without letters, units, blanks, or zeros).

IV. User Input Handling. The tool request a user to enter values of Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO). Also verified input value are not empty or zero. It also checks that HOMO and LUMO are not same.

V. Calculations of Chemical Properties. The program calculate this properties

Energy Gap, Ionization Energy, Electron Affinity, Hardness, Chemical Potential, Softness, Electrophilicity, Index hardness, Electronegativity.

Each result is printed both to the console and saved to the text file, with labels for clarity.

VI. Result output and Save option.

After calculations, the program closes the file. Also provide option for user to save the results. Enter to exit the program without using mouse option.

8. Conclusion

The current research focuses on designing and implementing an efficient software tool, developed HMG.A1, to minimize the time consumptive step of manually computing molecular properties from DFT log file. Thanks to the improved structure and the methods of calculations implemented in the tool, computational researchers are able to devote their time mainly on the visualization and interpretation of the results rather than bogging themselves down with the data. The paper also provides the future trend of Python usage, including the molecular modeling and analysis, and presents a lightweight, flexible tool for computational chemistry.

It would significantly improve the program's performance in computational chemistry if the visualization functions were incorporated and HMG.A1 was developed for mobile and Web applications. Despite the computationally constrained environment that may exist within the context of typical mobile personal computers, the effective use of external computational resources and Internet services may offer a reasonably efficient and more importantly, feasible method of conducting computations using typically advanced computational tools. Thus, meeting all these needs might help HMG.A1 become more universal and user-friendly for Computational Chemists.

Going forward, HMG.A1's potential for mobile platform expansion may improve its usability even further by enabling users to do first computations on portable devices. Users would also be able to do more complicated computations without requiring a lot of local hardware if cloud based computing resources are available. Future improvements might potentially include the ability to calculate molecular properties through voice assistance

Data availability

Permanent link to code/repository used for this code version:

https://github.com/aziz1sh1/HMG.A1

Permanent link to reproducible capsule. https://codeocean.com/capsule/9970901/tree/v1: DOI: 10.24433/CO.9753864.v1

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