THE CROSS-PLATFORM QUANTUM CHEMISTRY SOFTWARE FOR COLLEGE CHEMISTRY EDUCATION

Mengxin Song, Ping Guo
Image Processing and Pattern Recognition Laboratory, Beijing Normal University, Beijing 100875, China

Shi Peng
Institute of Educational Equipment Research, Ministry of Education, Beijing 100080, China

Keywords: Cross-Platform, Quantum Chemistry Software, Graphic User Interface (GUI), Chemistry Education.

Abstract: Quantum Chemistry is one of the most important fields in Chemistry. However, lots of the concept are too abstract to comprehend for college students. Consequently, how to aid the students in this field to gain an intuitionistic comprehension of the quantum chemistry related knowledge becomes a crucial problem. A cross-platform quantum chemistry software (SIMU) is introduced in this paper. With a friendly graphic user interface (GUI), SIMU can be used to help users to build molecular and display the visualized computing results. SIMU is particular designed for students as well as researchers in the field of quantum chemistry, they can easily accomplish their demanded computations with friendly GUI. A survey conducted on several quantum chemical labs with the experience of SIMU supported teaching and learning shows that it is of great assistance of understanding abstract quantum chemical concept and acceptance of the SIMU platform.

1 INTRODUCTION

Quantum Chemistry is one of the most important fields in Chemistry. Although quantum concept is at the heart of our understanding of modern chemistry, materials science, and emerging quantum technologies such as quantum computing, it has traditionally been difficult to comprehend (Dill, Crosby, Carr, Garik, AlexGolger, Hoffman and Horwitz, 2004). Wu, Krajcik, and Soloway (2001) found that visualizing tools may help students to understand the chemical representations. And with the development of computational quantum chemistry, more and more researchers and students in this field need to use computer software to support their research and learning. Compared to the traditional teaching and learning method, using visualization method to assist students to comprehend the concept of quantum chemistry has lots of advantages (Ye and Chen, 1999). Some researchers begin to focus on how to using the assistant tools to help the students to learn abstract concept (Miranowicz's, 2009). Before the appearance of the quantum chemistry software, students need to write the computation needed input files by themselves, but only the advanced users have the ability to generate the input files manually, the beginners or the students in this field might not be sure about how to write this input file. And another problem is that generating the file manually often leads to mistakes, and once the problems occur, it is inconvenient for the students to check out which part(s) in the file is(are) incorrect. The effectiveness of comprehending the abstract concept of the quantum chemistry is another problem the students encountered, without computer supported education tools, such as the visualized software, students can hardly imagine the computational result such as the molecular density distribution after the calculation. With the development of computer technology, the appearance of the cross-platform quantum chemistry software---SIMU can provide the learning tool to help students in this field to solve the above mentioned problems. Students can use the graphic user interface (GUI) to build molecular, then after the computation, they can get visualized computing results. Taking the advantage of the SIMU's friendly GUI, students can easily obtain the input files, and at the mean time, they can gain an intuitionistic comprehension of the abstract concept in quantum

Song M., Guo P. and Peng S. (2010).
THE CROSS-PLATFORM QUANTUM CHEMISTRY SOFTWARE FOR COLLEGE CHEMISTRY EDUCATION.
In *Proceedings of the 2nd International Conference on Computer Supported Education*, pages 438-441
DOI: 10.5220/0002793104380441

chemistry, such as density distribution. This is our motivation to apply computer graphics technique to develop education supporting tool for the assistance of college students to study the concept of quantum chemistry.

As a cross-platform software, SIMU can run on Windows, Linux and Macintosh. A commonly flow of using SIMU to do the quantum chemistry computational is: user first uses molecular builder to build their needed molecular, and then setting the computation parameters by using job generator module, finally the visualized results can be gotten through property viewer.

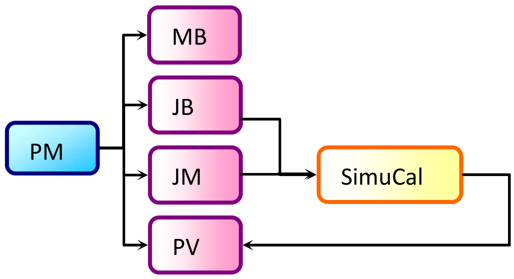

Figure 1: The relationship of the 6 main components in SIMU.

2 THE STRUCTURE OF SIMU

There are mainly six components in SIMU. (1) Project Manager (PM) is in charge of the management of the other five modules, and it is the highest level of the SIMU's structure, (2) Molecular Builder (MB) helps user to build molecular by GUI, (3) Job Generator (JB) helps user to generate the needed parameters for computation, (4) Job Monitor (JM) can monitor the status of the user's submitted jobs, (5) Property Viewer (PV) displays the computational results by using the graphic interface. (6) SimuCal is a quantum chemistry computational package. The relationship between these six modules is illustrated in figure 1.

As shown in figure 1, PM is in charge of the management of MB, JB, JM, PV, and SimuCal modules. So PM it is the most cardinal module in SIMU. After setting the parameters for computation, user can use SimuCal module to calculate while use JM to monitor the status of the submitted jobs. Finally, when the job finished, PV module will show the computation results by graphic interface.

3 THE MAIN COMPONENTS IN SIMU

In this section, we will introduction the 6 main components of SIMU respectively.

3.1 Project Manager (PM) Module

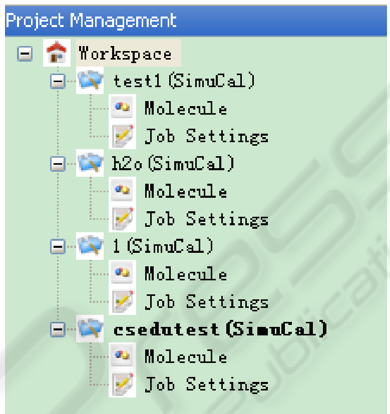

Figure 2: The interface of PM.

PM module is the most important module in SIMU. It is in charge of the management the other modules in SIMU. Users can use PM to management their projects. Figure 2 shows the interface of PM. We can see from figure 2 that SIMU's users can use the tree list of PM to management the created projects conveniently. This multi-task design brings lots of convenience to users, because the quantum chemistry software users often need to maintain several computational tasks, and PM module can help them to meet this requirement.

3.2 Molecular Builder (MB) Module

MB module helps users to build their demanded molecular by using a friendly GUI, as shown in figure 3. With this module, students can gain a more intuitionistic comprehension of the structure of molecular with the help of graphics tool. Also, students can use SIMU to build complex molecular, as it is shown in figure 4.

3.3 Job Generator (JB) Module

JB module helps students to set the computation needed information. Students can set the parameters through the JB dialog. After setting the parameters in this dialog, students can generate their own input file. It will be helpful to avoid the fault during manually generating the input file.

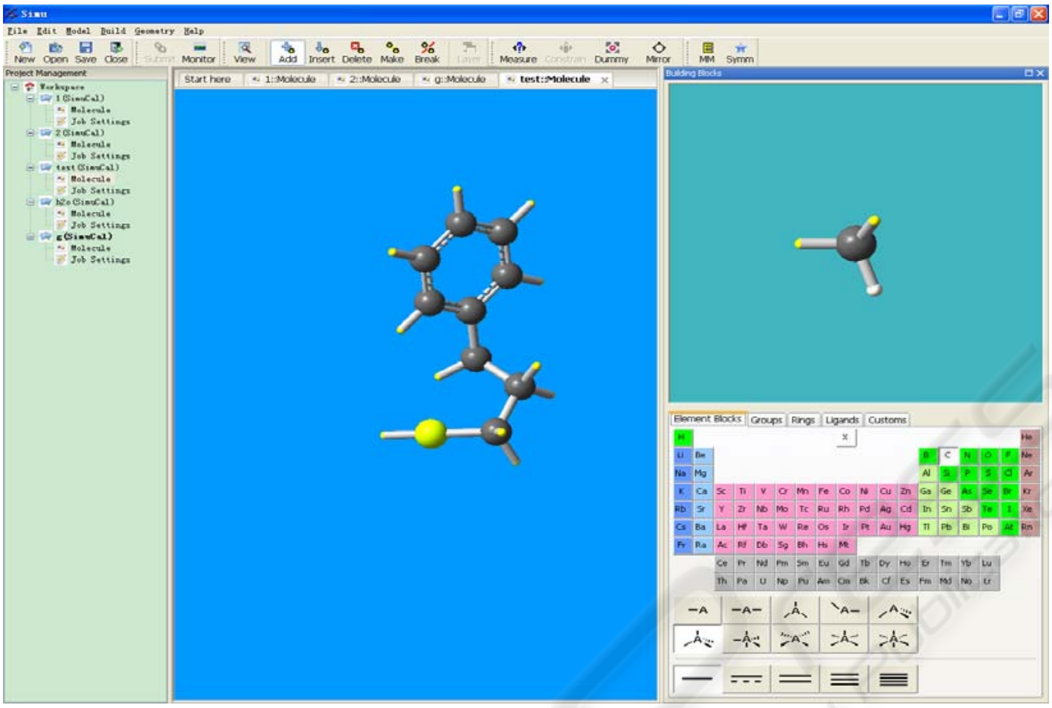

Figure 3: Using Molecular Builder (MB) module to build molecular.

3.4 Job Monitor (JM) Module

JM module helps user to monitor the submitted computation job, because quite a number of quantum chemistry job cannot finish in a few minutes, some jobs need to be computed for several days, so users need to know the current status of their submitted jobs.

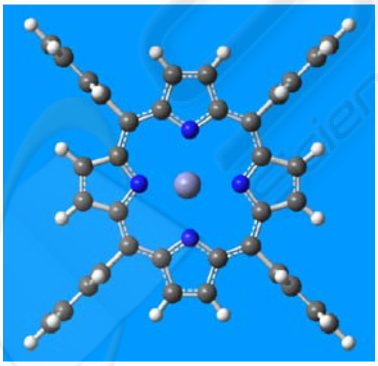

Figure 4: Using SIMU to build a complex molecular.

Consequently, we design the JM module in SIMU to meet the users' requirement in this aspect.

3.5 Property Viewer (PV) Module

PV module displays the finally computational results for users by graphic method. Figure 5 shows an example that users use PV to view the density of the

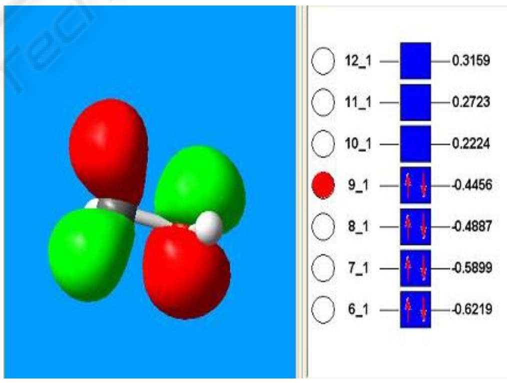

Figure 5: Using SIMU to display the density of the molecular after the computation.

molecular. PV also can display the molecular vibration status for the students. As we know, both the density and vibration of molecular are abstract concept which is difficult for students to understanding. However, with the assistance of SIMU software tool, students can gain an intuitionistic sense of the above concept and grasp the related knowledge more easily.

3.6 The Quantum Chemistry Computational Package SimuCal

There are several quantum chemistry computational packages, such as Molcas (Veryazov, Widmark, Serrano-Andre, Lindh and Roos, 2004). We also design and develop a quantum chemistry computational package for SIMU and call it as SimuCal. SimuCal contains several computational programs, it can help user to do the needed computations. SimuCal provides some basic computational methods, such as Semi-Empirical, Hartree-Fock, and MP2 (Coitiño, Ventura and Sosa, 1992). And SimuCal provides different job types for users, such as Single Point Energy, Gradients, Geometry Optimization, Transition State, Vibration Frequency, Opt-Freq, and Intrinsic Reactive Coordinates. Students can use JG module to select the job type and computation method to meet their need.

4 CONCLUSIONS

4.1 Discussions

SIMU is designed as a computer supported education tool to aid the students in the quantum chemistry field to accomplish their computations and to comprehend the abstract concept in this field. With the assistance of SIMU's GUI, students can easily understand the abstract concept of quantum chemistry, and gain the computer generated input files instead of manually generating them. As we know, till now there are several quantum chemistry software in the international market. However, China is a developing country, it is impossible to afford some commercial software such as GaussView as the teaching assistance tool for most universities in China. In order to meet the students' need for learning the related abstract concept and knowledge with visualized tool, we design and implement the cross-platform quantum chemistry software SIMU.

The price of SIMU is acceptable for college students in China, and the functions of SIMU can meet their study demand. With the help of SIMU's friendly GUI, college students surely can gain an intuitionistic comprehension of the quantum chemistry related knowledge.

4.2 Conclusions

We design and develop a cross-platform quantum chemistry software, SIMU. SIMU can be used to support college chemistry education, it aids the students in the quantum chemistry field to gain a intuitionistic comprehensions of the abstract concept and knowledge. At the mean time, SIMU also can be used as research assistant tool, which will bring lots of convenience for the researchers as well as students of the quantum chemistry field.

The graphic user interface of SIMU is very friendly, and in practical applications the operation of SIMU is stably. A survey we conducted on several quantum chemical labs with the experience of SIMU supported teaching and learning shows that it is of great assistance of understanding abstract quantum chemical concept and acceptance of the SIMU platform.

ACKNOWLEDGEMENTS

The research work described in this paper was fully supported by the grants from the National Natural Science Foundation of China (Project No. 20733002, 20873008, 60675011). Prof. Ping Guo and Shi Peng are the authors to whom the correspondence should be addressed.

REFERENCES

Coitiño, E., Ventura, O. and Sosa, R. (1992). Comparative ab initio and semi-empirical study of hydrogen bonded complexes of NH_3 and H_2O. *Journal of Molecular Structure: THEOCHEM.* 254, 315-328.

Dill, D., Crosby, A., Carr, P., Garik, P., AlexGolger, Hoffman, M. and Horwitz, P. (2004). Designing targeted interactive software for chemical education for multiple educational environments. *ACS 227th National Meeting.*

Miranowicz, N. and Miranowicz, M. (2009). Chemistry education with podcasts. Strategy and effectiveness. *Research, Reflections and Innovations in Integrating ICT in Education.* 1, 338-341. Formatex.

Ye, Q. and Chen, Y. (1999). The computer multimedia application in college chemical education. *University Chemistry*. 39~41. (in Chinese).

Veryazov, V., Widmark, R.O., Andre, L., Lindh, R. and Roos, B. (2004). 2MOLCAS as a Development Platform for Quantum Chemistry Software. *International Journal of Quantum Chemistry,* 100, 626-635 .

Wu, H., Krajcik, J.S. and Soloway, E. (2000). Promoting conceptual understanding of chemical representations: students' use of a visualization tool in the classroom. *Journal of research in science teaching.* 38, 821-842.