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Enhancing Molecular Modelling Skill of High Schools Chemistry Teacher using Computational Chemistry Training

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Abstract: Current developments in information and communication technology require innovative efforts to integrate computers and visualization in learning. In the field of chemistry, many studies have proven that the integration of ICT plays a significant role in increasing the effectiveness of chemistry learning. The aim of this workshop activity is to increase the knowledge and skills of high school/MA chemistry teachers in Lampung Province in teaching atomic structure and chemical bonding based on computational chemistry using computational chemistry applications. This activity will be carried out for 6 months and will be attended by high school/MA chemistry teachers in Lampung Province. The training methods that will be used are workshops and guided practice. The activity evaluation design was carried out in 2 ways, namely evaluating participant understanding and evaluating participant skills. Evaluation of participants' understanding is based on pretest scores at the beginning of the activity and posttest at the end of the activity. Evaluation of participant skills is based on the participant performance assessment criteria during the workshop process. The results of the service implementation show that participants have been able to understand and know the types, advantages, functions and working/working procedures of smartphone-based molecular modeling applications for learning chemistry on atomic structure and the periodic system of elements. The participant performance during the training increase significantly in operating the computational program. The follow-up to this service is to expand the service participants to all teachers in Lampung Province and expand the workshop material not only on atomic structure and the periodic system of elements, but on other material such as chemical bonds, reaction rates, equilibrium, and so on.

Keywords: computational chemistry training, molecular modelling skill, high school teacher.

▪ INTRODUCTION

The development of information and communication technology (ICT) has changed student learning patterns. Millennials want to learn things differently, quickly, and tend to lack the patience to read books, even though we believe it's the only way to learn new information. Some of these kids rarely even open their books before exams, sometimes even before the end of the semester. They will search for answers and concepts online (generally using the Google search engine), regardless of the accuracy and correctness of the answers (Abouserie et al., 1992).

Chemistry as a natural science has the characteristics of an abstract field of science, involving spatial and mathematical thinking abilities so that many students are less interested in chemistry. Apart from this fact, chemistry is a science that is at the center of technology and engineering in various fields, and is easy to apply to real life (Kyle et al., 2011). For example, understanding basic chemical concepts is necessary to solve the energy crisis, to develop environmentally friendly production and waste management methods, to detect biological weapons in real time, to develop better pharmaceutical

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drugs, to solve environmental problems, and to design new nanotechnological functional materials (Boyce & Bertozzi 2011).

With the new dilemmas and challenges brought by this new generation of learners, chemistry learning must also be able to adapt to developments in ICT, especially now that the world is entering an era of digitalization called the Industrial Revolution 4.0 era. For example, most of them now have many gadgets and most of their time is spent browsing online for social or entertainment purposes. Currently, ICT is widely used for purposes such as distance learning, podcasts, mini-videos, streaming, social media, PowerPoint, and transparency (Stefl-Mabry, 2010).

One area in chemistry that takes advantage of ICT developments is computational chemistry and 3D molecular visualization which is used as a molecular modeling tool. Computational chemistry and 3D molecular visualization tools are generally used as tools to help students understand difficult and abstract concepts and as tools for advanced chemistry or scientific research. By using computational assistance and chemical visualization, students will more easily understand the shape and structure of chemical molecules in 3 dimensions. Computational chemistry is a branch of chemistry that uses computer simulations to assist in solving chemical problems. In its application, computational chemistry uses theoretical chemical methods incorporated into computer programs, to calculate the structure and properties of molecules and solids (Tetko et al., 2005; Chatfield, 2002). This is necessary because, apart from relatively recent results regarding the molecular hydrogen ion (dihydrogen cation, see references therein for more details), the quantum many-body problem cannot be solved analytically, let alone in closed form. While computational results usually complement the information obtained by chemical experiments, in some cases they can predict hitherto unobserved chemical phenomena.

Examples of such properties are structure (i.e., the expected positions of the constituent atoms), absolute and relative (interaction) energies, charge distribution of electronic charges, dipole and higher multipole moments, vibrational frequencies, reactivity, or spectroscopic quantities. others, and cross-sections. for collisions with other particles. The methods used include static and dynamic situations. In all cases, computer time and other resources (such as memory and disk space) increase rapidly with the size of the system being studied (Young, 2004). The system can be a single molecule, a group of molecules, or a solid. Computational chemistry methods range from very approximate to very accurate; the latter is usually feasible for small systems only. Ab initio methods are based entirely on quantum mechanics and fundamental physical constants. Other methods are called empirical or semiempirical because they use additional empirical parameters (Lewars, 2003).

Both ab initio and semi-empirical approaches involve approaches. These range from simple forms of first principles equations that are easier or faster to solve, to approximations that limit the size of the system (e.g., periodic boundary conditions), to fundamental approximations to the underlying equations that are required to reach any solution to them at all. For example, most ab initio calculations make a Born-Oppenheimer approximation, which greatly simplifies the underlying Schrödinger equation by assuming that the core remains in place during the calculation. In principle, ab initio methods eventually converge to an exact solution of the underlying equation as the number of approximations decreases. In practice, however, it is impossible to eliminate all approximations, and residual errors inevitably remain. The goal of

computational chemistry is to minimize this residual error while maintaining workable calculations (Lipkowitz, Cundari, Boyd, 2008).

In some cases, the details of the electronic structure are less important than the long phase space behavior of the molecule. This is the case in thermodynamic studies of protein conformation and protein–ligand binding. Classical approaches to potential energy surfaces are used, because they are computationally less intensive than electronic calculations, to allow longer simulations of molecular dynamics. Furthermore, cheminformatics uses more empirical (and computationally cheaper) methods such as machine learning based on physicochemical properties. One of the typical problems in cheminformatics is to predict the binding affinity of a drug molecule to a given target (Lipkowitz, Cundari, Boyd, 2008; Manly, Louise-May, & Hammer, 2001).

The term theoretical chemistry can be defined as a mathematical description of chemistry, while computational chemistry is usually used when mathematical methods are sufficiently well developed that they can be automated to be implemented on a computer. In theoretical chemistry, chemists, physicists, and mathematicians develop algorithms and computer programs to predict atomic and molecular properties and reaction pathways for chemical reactions. Computational chemists, in contrast, may simply apply existing computer programs and methodologies to specific chemical questions (Manly, Louise-May, & Hammer, 2001).

Conditions in the field, especially high school chemistry teachers in Lampung Province, are still unfamiliar with 3D molecular visualization. Based on the results of exclusive interviews with chemistry teachers in Lampung Province, the majority of respondents stated that they had never heard of and utilized computational chemistry programs or 3D molecular visualization to help them in their learning activities. The learning carried out still relies on blackboards and conventional lectures in front of the class. The use of 3D molecular visualization in chemistry learning is still very rare. The aim of this training were to increase knowledge about computational chemistry and molecular visualization of high school chemistry teachers in Lampung Province and improve their skills in operating computational chemistry software and molecular visualization using computational chemistry applications.

▪ METHOD

The computational chemistry training method for state and private high school chemistry teachers in Lampung Province is carried out through several steps, including: lecture, workshop, personal activities, presentation, implementation. Lecture activity was carried out at the beginning of the activity, carried out by the lecturer, to provide insight to chemistry teachers about chemical computing and visualization and their application in learning chemistry in the classroom. At the end of the lecture, the lecturer provided examples of innovative learning with the help of computing and chemical visualization. After the participants gain insight into how to carry out computational chemical calculations and 3D molecular visualization, then in groups, the participants were trained to complete chemical calculation cases to prove chemical theories and phenomena accompanied by lecturers and students. Workshops were also held to create learning tools based on computational chemistry and 3D molecular visualization. Teachers carry out computational calculations and visualization of other chemical objects independently in their respective homes (each teacher gets certain Basic Competencies that have been determined by the lecturer. This independent activity is still accompanied by the lecturer, either through direct visits or consultation via email. Teachers present the work that has

been created independently, then criticized by colleagues, and given input by the lecturer. Teachers implement computational chemistry and molecular visualization in learning, then report the results.

The institutions involved in this research are the University of Lampung, in this case represented by LPPM Unila, chemistry teachers group in Lampung Province, and the home schools of the trainee teachers. The role of LPPM Unila is to facilitate training activities in the form of funds, the role of teachers group is to facilitate training activities at teachers group meetings, the role of schools is to give permission for chemistry teachers to take part in training, and specifically High School Bandar Lampung provides a place for carrying out training activities. Evaluation is carried out at the initial stage of the activity in the form of a pre-test, at the end of the activity in the form of a post-test and performance assesment by presentation. Pretest and posttest material includes knowledge about chemical computing and visualization. Criteria for success in activities include post-test scores. Training activities are declared successful if at least 80% of participants obtain a post-test score ≥ 75.

▪ RESULT AND DISCUSSION

Computational chemistry training in teaching atomic structure and chemical bonds for chemistry high school teachers has been carried out at FKIP Lampung University. Participants consisted of 15 teachers from 3 districts in Lampung, namely Metro, Kotabumi and Bandar Lampung. This activity begins with giving a pretest to test participants' understanding regarding the application of computational chemistry and its role in supporting the chemistry teaching and learning process in schools, especially regarding atomic structure and quantum mechanics. The questions asked to participants included (a) what media do teachers use when teaching atomic structure and chemical bonds?, (b) have teachers ever used ICT-based learning media when teaching atomic structure and chemical bonds? If yes, what kind of media have you used? (c) What difficulties have you experienced when studying atomic structure and chemical bonds? (d) In your opinion, how important is the use of visualization applications in studying atomic structure and chemical bonds?.

Participants' answers showed that several media such as molymod, static images from textbooks, Colorado phet simulation applications, YouTube videos, LKPD, had been used by participants although there were still many (39%) participants who had not used chemical visualization and computational applications or software. The applications that have been used include phet simulation, chemsketch, and Android-based atom visualizer. Some of the difficulties faced by teachers when learning atomic structure and chemical bonds include students' difficulty in understanding abstract concepts of atomic structure and chemical bonds, students have difficulty predicting compounds that are formed as a result of the formation and breaking of chemical bonds, teachers have difficulty in making lessons fun and easy to understand, teachers' difficulties in visualizing atomic structures and chemical bonds.

After identifying the difficulties experienced by teachers when teaching material about atomic structure and chemical bonds, participants (teachers) were introduced to several chemical computing applications that were run via Android phones or laptops/PCs. Some of these applications include Atom visualizer, V-SEPR and WebMO (via Android cellphone) while applications that can be run from a laptop/PC include Avogadro, Gabedit and WebMO demo server. The training material presented includes the Bohr atomic model and quantum mechanical atomic model for simple elements in the

periodic system using the Atom application. The appearance of the application can be seen in Figure 1.

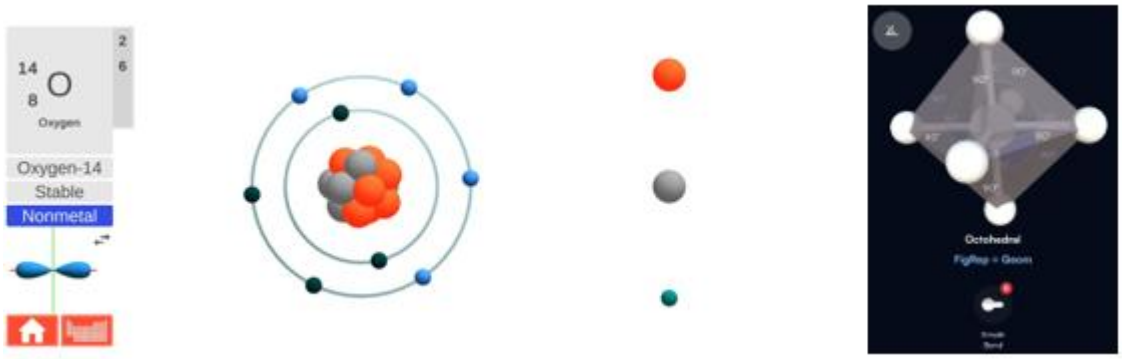


Figure 1. Visualization of Bohr atomic model and tetrahedral VSEPR

The use of computational chemistry applications continues in the material of the periodic system of elements and the periodic properties of elements. For this material, the WebMO demo server application (Laptop/PC) or the Android version of WebMO is used. The periodic properties of the elements discussed are the tendency of atomic radius and ionization energy of element atoms in one group and period. The display of the Webmo application used in learning the periodic properties of elements can be seen in Figure 2.

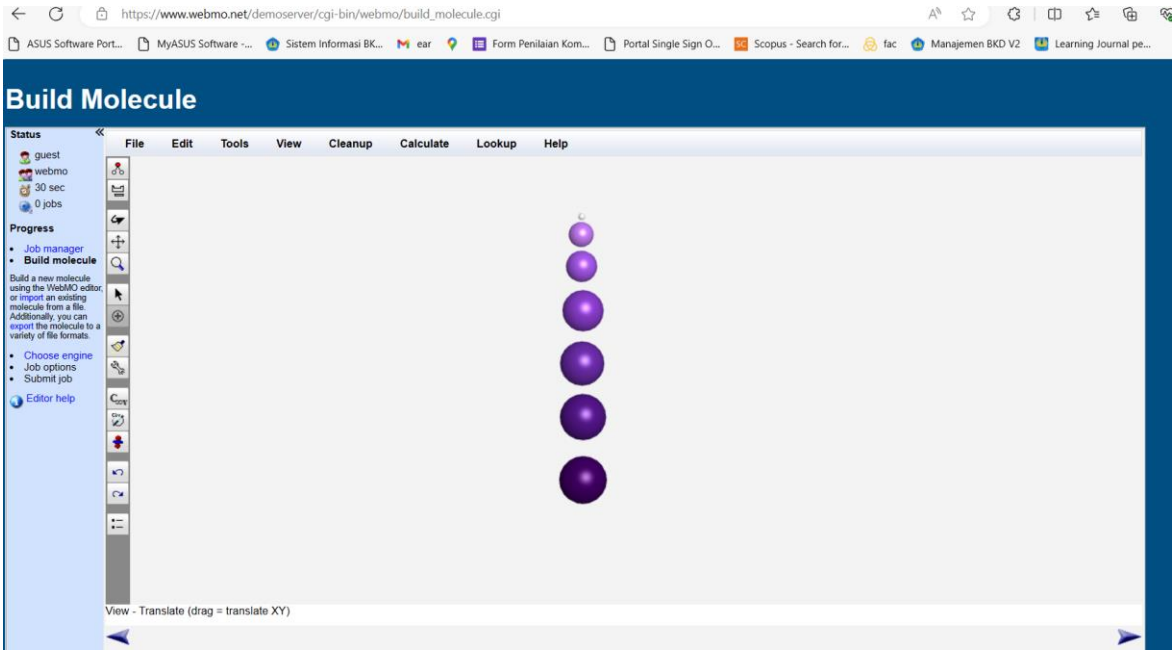


Figure 2. Display of the Webmo application used in learning the periodic properties of elements

Furthermore, the trend in the ionization energy of atoms of elements in one group is also studied in this training. In theory, the ionization energy of atoms of elements in a group from the top element to the bottom will become smaller, which is related to the amount of energy needed to remove one outer electron in a gaseous state. This

phenomenon can be proven by chemical computational experiments using Huckel orbital energy calculations provided by the WebMO application. Display of the Huckel orbital energy calculation results and ionization energy trend graph is shown in Figures 3.

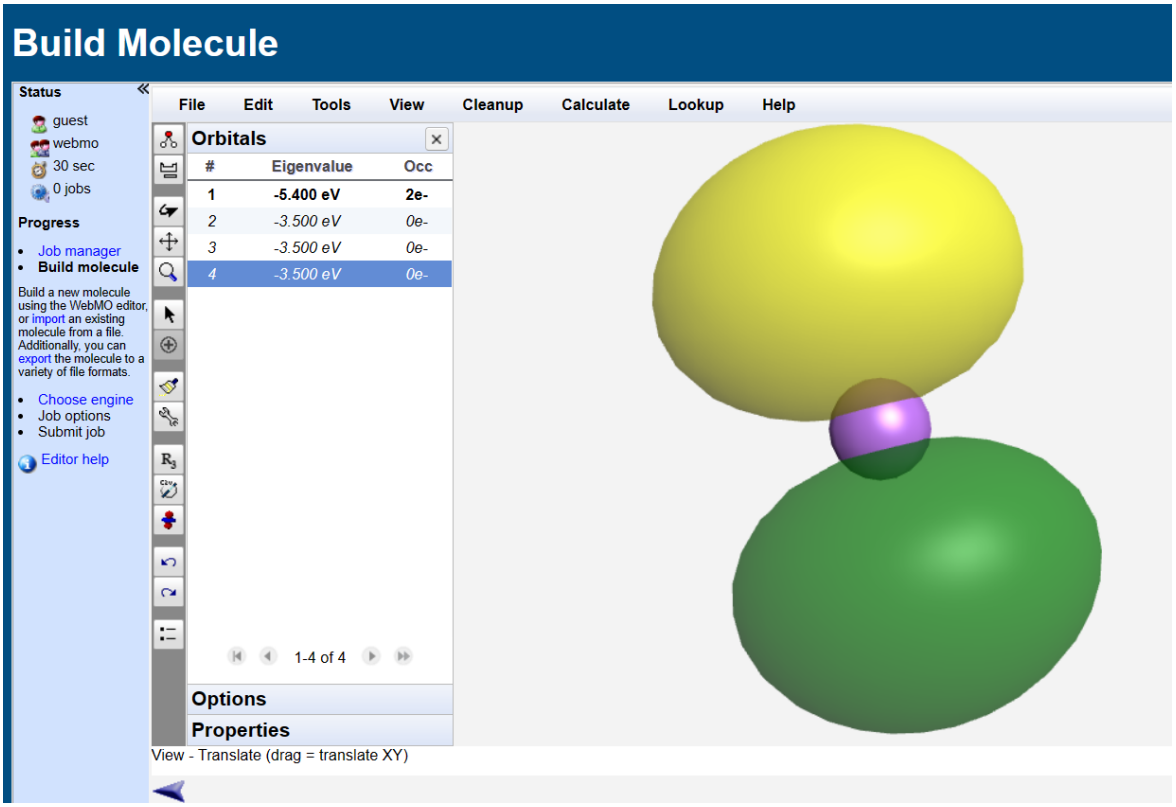


Figure 3. The display of Huckel orbital energy calculation in WebMo application

The utilization of computational chemistry applications is implemented through demonstrations and group work. Participants in each group are given assignments and outlines to visualize and calculate the properties of molecules and/or atoms regarding atomic structure and the periodic system of elements. The demonstration and group work of service participants can be seen in Figure 4 and 5.



Figure 4. Participants received the lecture



Figure 5. Participants run the computational chemistry software guided by the lecturer

After the training is carried out, participants are also asked to take a post-test with the same questions as the pre-test to measure the impact of their service. The results showed that the average of post-test score was 80, and there were no participant get post

test score under 75 as showed by Figure 6. It showed that all participants were able to answer the post-test questions well as demonstrated by knowing and understanding the working procedures of smartphone-based molecular modeling applications and the various types and advantages of these applications.

Besides the post-test, the skill of participant in operating the program was assessed by performace test in form of assignment presentation. The representatives from the participants presented the results of the assignment in creating learning media on the topic of atomic structure and chemical bonds using the WebMo program based on computational chemistry and then commented on by the other participants in turn. As a result, all participants were able to create learning media using the computing program. The training then continued with online assistance at home to create complete media on atomic structure and chemical bonds. Based on the result the implementation of the service took place effectively and was able to increase the understanding and skill in using computational chemistry program of the service participants.

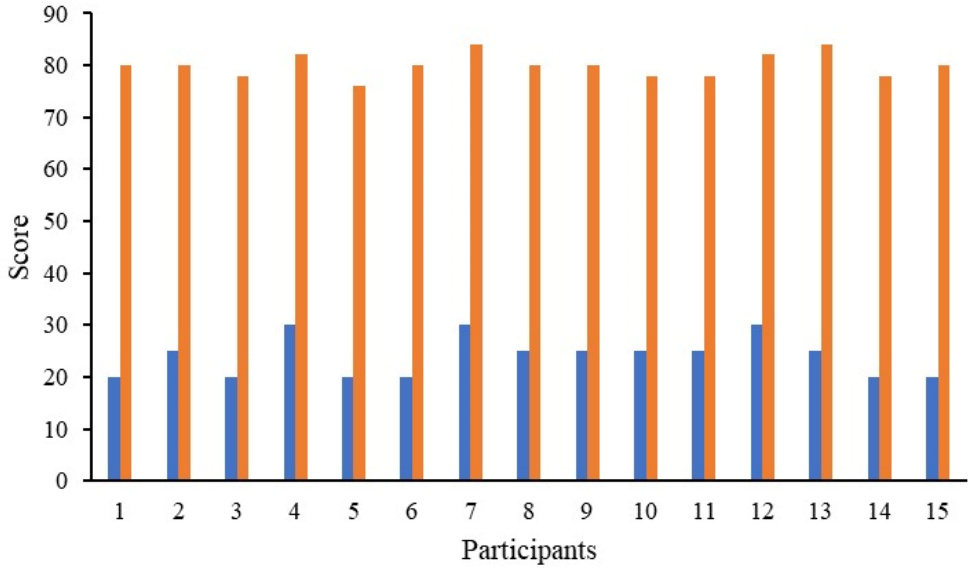


Figure 6. Pretest (blue) and posttest (orange) scores of participants

▪ CONCLUSION

The results of the service implementation can be concluded that the participants have been able to understand and know the types, advantages, functions and working methods/work procedures of chemical computing-based applications for learning chemistry on atomic structure and the periodic system of elements. Participants' ability to use computational chemistry applications also increased, as indicated by increased skills in operating the program in creating learning media on the topic of atomic structure and chemical bonds. The follow-up to this service is to expand the service participants to other districts in Lampung Province and expand the workshop material, not only on atomic structure and the periodic system of elements, but on other materials such as chemical bonds, reaction rates, equilibrium, and so on.

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