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Cite as: AIP Conference Proceedings **2638**, 090003 (2022); https://doi.org/10.1063/5.0104013
Published Online: 18 August 2022

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Developing Computational Chemistry Laboratory Work Module for Dye-Sensitized Solar Cells

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Abstract. This study aims to determine the validity, practicality, and effectiveness of the newly developed computational chemistry-based laboratory work module. The developed laboratory work module is applied to test lawsone's efficacy and its derivatives as a sensitizer in dye-sensitized solar cells DSSC. The Design and Development D&D research model is used at every stage of development. The research population was 90 prospective teachers of chemistry education, Faculty of Teacher Training and Education, University of Mataram, Indonesia. All population has passed computational chemistry and photochemistry courses in the 2020/2021 academic year. The research sample was 40 prospective teachers, with a comparison of computational chemistry and photochemistry class samples was 3:1, where the sample was taken randomly. Test the validity of the laboratory work module conducted by three expert validators. The Aiken index shows 0.88, and the developed laboratory work module is in the high validity category. The practicality test was carried out by distributing response questionnaires to prospective teachers. The practicality test score is 82%, which indicates that the practicality of the module is categorized as very practical. Furthermore, the module effectiveness test is carried out by asking respondents to answer the questions provided in the module. The average score obtained by prospective teachers is 71.6% which indicates that the application of the module can improve the understanding of the concept of prospective teachers. In conclusion, the laboratory work module based on computational chemistry is valid, practical, and effective. Modules can be used as reinforcement in learning in computational chemistry and photochemistry courses.

INTRODUCTION

Chemistry requires a student to understand the concept and practical aspects of learning chemistry [1,2]. Students can succeed in learning chemistry if they can explore their learning experience more broadly. One of the ways to do this is through laboratory work activities [3-5]. According to the cone experience theory from Edgar Dale, the learning process carried out through direct experience will make the learning process concrete, and students can remember 70% of what is said and done in real time. When an educator provides many skill-based activities, students will understand them effectively and efficiently [6-10].

The implementation of chemical laboratory work faces various obstacles. Our observations show that several factors cause chemical laboratory work to be rarely carried out on the islands of Lombok or Indonesia. These factors include the limitations of chemicals. Since the Bali bombings, the price of chemicals has increased by 200%, and it is difficult to obtain specific materials. The time to prepare laboratory work is relatively long. It makes laboratory work rarely done. Lack of availability of laboratory work tools and a high level of risk for chemical laboratory work in the laboratory (such as explosions or chemical poisoning), and obstacles in managing waste generated from laboratory work. In addition, there is no standard laboratory work module that is ready to be used [11,12].

The laboratory work module is made as attractive as possible and makes it easier for students in the laboratory work process. One of the things that make laboratory work interesting to do is interesting content in laboratory activities. The use of computational chemistry in laboratory work is quite interesting for students [13-14]. However, the availability of laboratory work modules for computational chemistry courses in Indonesia is still very lacking.

The 9th International Conference of the Indonesian Chemical Society ICICS 2021
AIP Conf. Proc. 2638, 090003-1–090003-7; https://doi.org/10.1063/5.0104013
Published by AIP Publishing. 978-0-7354-4380-8/$30.00

Laboratory work will directly make students' understanding of computational chemistry more optimal. A computational chemistry laboratory work module will also enable students to work independently and construct their knowledge through each instruction presented in the module [15-16].

Computational chemistry can answer laboratory work problems that are rarely carried out in laboratories. The method used in computational chemistry is very flexible, and almost all practical chemistry materials from simple to high difficulty levels can be modeled well. The availability of various kinds of computational chemistry software for free is also something that must be utilized. In addition to the low cost of laboratory work, computational chemistry methods have other advantages such as a high level of accuracy, shortening practice time, safe, and can undoubtedly help improve understanding of chemistry optimally [17-20].

In the development of laboratory work modules, we focus on the dye-sensitized solar cell module. The study of solar cell energy is fascinating because it is an essential topic related to alternative energy sources. In addition, most of the prospective teachers who will be sampled for the practicality test of the module come from areas that lack electrical energy. This condition will encourage their interest in studying aspects of solar cells from the perspective of computational chemistry. The availability of abundant sources of DSSC sensitizers in the tropics is also a driving force for the development of modules directed at solar cells based on natural products. Among the natural products for DSSC are various natural dyes that can be used. Lawsone is an example of a natural pigment used as active material in dye-sensitized solar cells. It has a conjugated structure so that lawsone has active properties that can be utilized as a dye sensitizing agent [21-23]. Based on this, a laboratory work module was developed based on computational chemistry to test lawsone's effectiveness and its derivatives as a sensitizer in dye-sensitized solar cells.

RESEARCH METHODOLOGY

The research was conducted in the 2020/2021 academic year, starting from the preparation stage in February to August 2021 at the Chemistry Education Study Program, FKIP, Mataram University. The type of research is development research that uses the development research model proposed by Richey and Klein [24,25]. The laboratory work module based on computational chemistry that was developed chose to test lawsone's effectiveness and its derivatives as a sensitizer in dye-sensitized solar cells. The laboratory works module used is based on the Hyperchem 6.0 application. There are at least six stages in the D&D model, each of which is a refinement of Hevner et al. [26], who previously explored the stages of the D&D model. The steps of the D&D model include: 1) problem identification; 2) describing the goal; 3) product design and development; 4) product trial; 5) evaluation of trial results; 6) communicating the test results.

The population in this study were 90 teacher candidates who were in the final year of chemistry education, Faculty of Teacher Training and Education, University of Mataram, who had passed the computational chemistry course and photochemistry class for the 2020/2021 academic year. The sampling technique is non-probability sampling by taking samples by giving a certain quota or quorum to a group [27]. The sample is 40 prospective teachers divided into two sample groups; namely, 30 respondents are taken based on the scores obtained by these students in the computational chemistry course, and 10 respondents are taken from students who have passed the photochemistry course. The research instruments are in the form of validation sheets, practicality, and effectiveness test questions. The validity analysis uses the Aiken V index, while the practicality analysis uses the practicality index. Furthermore, the description test was used to determine the effectiveness of the module.

RESULTS AND DISCUSSION

The first step for developing the module is to identify the problem. Problem identification was conducted by looking at the learning conditions, especially computational chemistry and photochemistry courses in the Chemistry Education Study Program, University of Mataram. After completing a needs analysis, it was found that there is no standardized laboratory work module, especially in the computational chemistry course as a compulsory subject, and it requires laboratory work in the learning process. Developing a laboratory work module that can support laboratory work activities in computational chemistry courses is necessary. The module needs to be made in Indonesian so that it is easy for students to understand. The topic for the module is dye-sensitized solar cells from natural materials because the subject is interesting. Lawsone and its derivatives were chosen because they are colored and good at absorbing light, and many studies have reported using lawsone compounds as sensitizers. The experimental test reports of lawsone and its derivatives are used as the basis for developing the module.

The next step is describing the objectives. The purpose of developing this laboratory work module is to fulfill the need for teaching materials in computational chemistry courses in the form of a laboratory work module based on computational chemistry. The research aims to develop a laboratory work module based on computational chemistry to test lawsone's effectiveness and its derivatives as a sensitizer in dye-sensitized solar cells. It is hoped that with this module, students are familiar with the methods contained in computational chemistry and know their application in real life. Specifically, this research aims to determine the validity, practicality, and effectiveness of the modules made.

Design and develop the artifact was conducted after identifying the problem and describing the research aims. This step consists of determining the format of the laboratory work module and preparing the initial product design, such as the module cover and module content. Most of the modules have been compiled at the design stage, but improvements are needed to achieve optimum teaching materials. At the design stage, an initial design of the laboratory work module is produced, which is referred to as prototype 1. This stage starts from making an initial design of the laboratory work module before being tested by experts, which consists of determining the module writing format and the design of the cover and content of the module.

At the development stage, what was done was to develop a chemical laboratory work module based on computational chemistry on dye-sensitized solar cells designed. The steps in this stage are to validate and revise the validation results. In this study, the development stage in question is the validity test. At this stage, the researcher asked the experts for theoretical consideration regarding the validity of prototype 1. The validator was asked to validate the laboratory work module both in terms of graphics, presentation, content or material feasibility, and linguistic aspects that had been produced at the design stage (prototype 1). At this stage, the validator examines the module that has been generated (prototype 1). Suggestions from the validator are used as a basis in revising the module resulting from the development carried out. After the laboratory work prototype 1 module was modified, the laboratory work prototype 2 module was obtained.

A brief picture of the laboratory work modules prototype 2 can be seen in Table 1. Prospective teachers are directed to relate the parameters of quantum chemistry to the DSSC parameters of lawsone and its derivatives. Prospective teachers are expected to have initial operating software skills and understand computational chemistry method selection techniques to obtain quantum parameters. Initially, prospective teachers will be directed to choose the molecular mechanics method, then semi-empirical, and then ab initio. It is done so that prospective teachers can select a method by the system being studied. After obtaining several quantum parameters, as shown in Table 1, prospective teachers are asked to graph the correlation between the quantum parameters and the experimental data. Then they were directed to determine which lawsone derivative was the best as a DSSC.

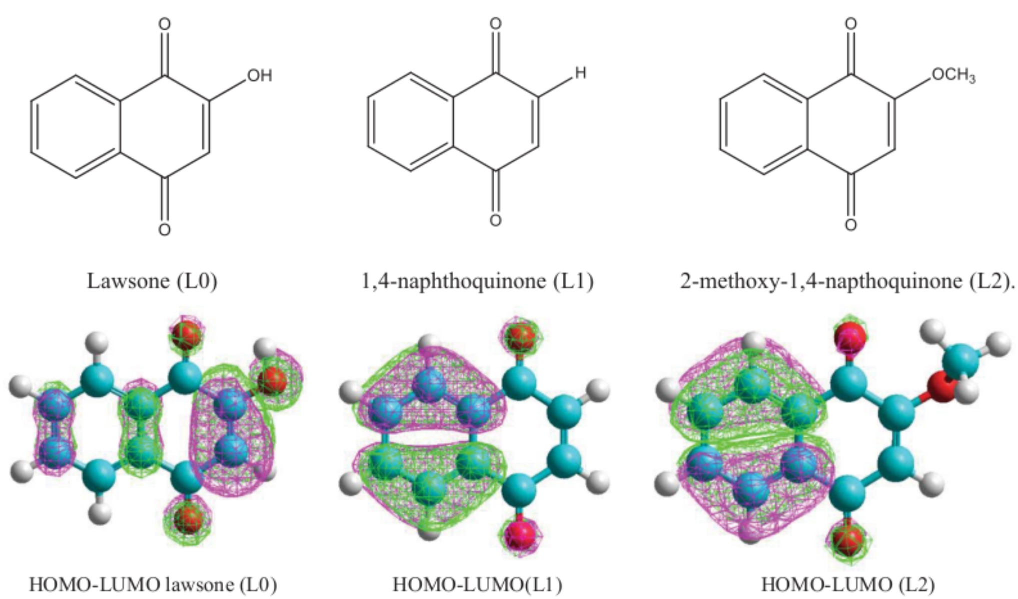

FIGURE 1. Lawsone and its derivatives; a. lawsone's 2D structure. b. lawsone HOMO-LUMO visualization

Subjecting the module product to testing is the next step. Product trials was conducted to determine the level of practicality of the developed modules. The product trial was carried out by 40 prospective teachers of the Chemistry Education Study Program, FKIP, University of Mataram. The results of product trials by students are then referred to as prototype 3. Suggestions from students are also considered for module improvements. The tests carried out included modules and practicality questionnaires related to the chemistry laboratory work module based on computational chemistry in the developed DSSC.

TABLE 1. Quantum parameter question table from laboratory work module.

Compounds	E_{HOMO}	E_{LUMO}	Ionization potential	Electron Affinity	Electronegativity	E_{gap} Theory	E_{gap} (Exp)
L0	-7.050	-3.265	7.050	3.265	5.157	3.785	2.47 eV
L1	-7.196	-3.261	7.196	3.261	5.228	3.935	
L2	-6.780	-3.177	6.780	3.177	4.979	3.603	

After the subject of the artifact to testing step is passed, the next step is to evaluate the testing results. Evaluation is carried out based on data obtained from expert and student responses that have been collected for later analysis. The data analysis carried out includes expert validation analysis, analysis of limited trial results, and analysis of the effectiveness of the developed module. Expert validation analysis data include validity and reliability analysis taken from assessments by experts related to the developed laboratory work module. In contrast, limited trial analysis data is taken from assessments by respondents, in this case, prospective teachers, FKIP, the University of Mataram who were selected as samples study. The analysis of the module's effectiveness is taken from the results of respondents' answers related to the questions made in the developed module. At the evaluation stage, suggestions from experts and respondents are considered for module improvement. At this stage, the product in the form of a laboratory work module based on computational chemistry to test the effectiveness of lawsone and its derivatives as a sensitizer in dye-sensitized solar cells has been completed.

Data analysis to measure the validity of the module is to use the Aiken index (V) with a value range of 0.4 to 1. The laboratory work module category is categorized as less valid if the V value is less than 0.4; valid category if the value of V is in the range of 0.4-0.8; and the category is very valid if the value of V is in the range of 0.8-1. Aspects assessed in the validation of the laboratory work module contain 21 statements about the module which generally include: (1) graphic aspects, (2) presentation aspects, (3) content feasibility aspects, and (4) linguistic aspects. The graph of the validity of the computational chemistry-based chemistry laboratory work module for testing the effectiveness of lawsone and its derivatives as a sensitizer in dye-sensitized solar cells can be seen in Figure 2.

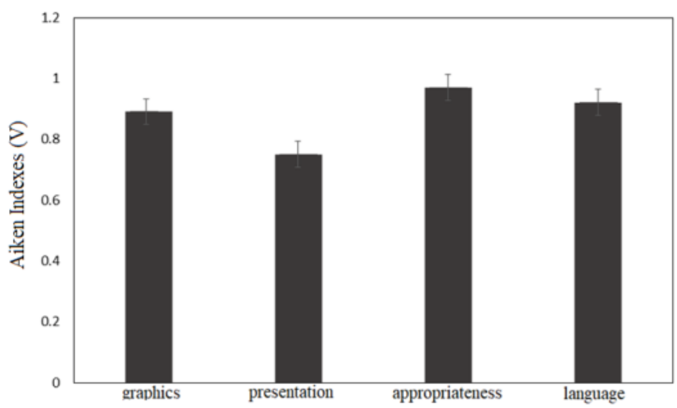

FIGURE 2. Validity of the laboratory work module

Figure 2 shows that each aspect of the assessment can be categorized as being in the range of valid and very valid criteria. It can be seen from the value shown by each aspect. The Aiken index for graphics, presentation, appropriateness of module content, and language are 0.89, 0.75, 0.97, and 0.92, respectively. The four aspects of the assessment module show valid values. The results of data analysis were obtained from the four aspects assessed. The aspect that received the lowest score was the presentation aspect. The modules created require good literature sources, which are then completed at the module development stage.

Data analysis to measure the practicality of the developed module uses a scoring system based on a Likert scale that has been modified with alternative answers, namely a score of 5 for highly practical; score 4 for practical; score 3 for quite practical; score 2 for impractical; score 1 for highly impractical. This product trial was conducted to determine the level of practicality of the developed module by distributing a module practicality sheet consisting of 14 statements about the laboratory work module, which contains four aspects, namely aspects of attractiveness, use, implementation time, and benefits of the module. The practicality category used is by grouping the values according to the practicality category in Table 2 [28].

TABLE 2. Practicality categories

No	Percentage	Categories
1	80% < x ≤ 100%	highly practical
2	60% < x ≤ 80%	practical
3	40% < x ≤ 60%	quite practical
4	20% < x ≤ 40%	impractical
5	0% < x ≤ 20%	highly impractical

The practicality of the module questionnaire analysis can be seen through the final scores carried out by 40 prospective teachers. The respondents of this study came from two classes, namely the computational chemistry class and the photochemistry class. It is done so that the module can be used for the general public, not only for students studying computational chemistry. The results of student respondents on the practicality of laboratory work modules based on computational chemistry to test the effectiveness of lawsone and its derivatives as sensitizers in dye-sensitized solar cells can be seen in Figure 3.

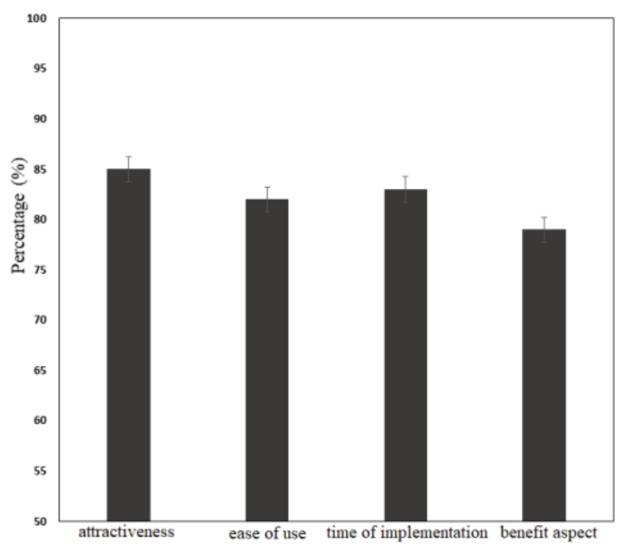

FIGURE 3. Practicality of the laboratory work module

Figure 3 shows that each component of the assessment can be categorized as being in the practical and very practical range. It can be seen from the value indicated by each component. The results of the practical analysis obtained from the four aspects are 85%, 82%; 83%; and 79%, respectively. Practical analysis of the four aspects of the module is considered to be highly practical and practical. It can be seen from the three aspects measured, namely the attractiveness of the module, the ease of use of the module, the time of implementation of the module, showing a value in the range of 80%-100%, which means the module is in the very practical category. The beneficial aspect of the developed module offers a value in the range of 60%-80%, which means the module is in the practical category. It happens because respondents feel they still lack the explanation of the theory described in the module. Most respondents suggested adding the basic theory used to make the modules easy to understand.

The theoretical basis developed by the author is made more concise so that users can construct their understanding so that aspects of the user's critical thinking can be formed. The author does not display too many explanations that can confuse users and search for additional literature on their own. Still, the author only writes down the points of the material discussed. Suppose the user wants to have a deeper understanding of the material in the laboratory work. The user can refer to the sources the author has listed in the module so that the user does not search again from the beginning related to the subject matter to understand the material. However, the results of the average total score for the practicality test of the module show a figure of 82%, which means that the module is in the very practical category to use.

The module's effectiveness is carried out by assessing the laboratory work of the respondents related to the demands requested in the module. The module requires students to complete observational data, draw the compound being tested, and answer five laboratory work questions to improve module users' critical thinking. Comparison of the assessment of the three aspects of each is 2:1:3. The results of data analysis showed that the average total effectiveness of the developed module was 71.6%, which indicates that the developed module is in the effective category for improving concept understanding. The results of the analysis of the module's effectiveness developed by 40 respondents can be seen in Figure 4.

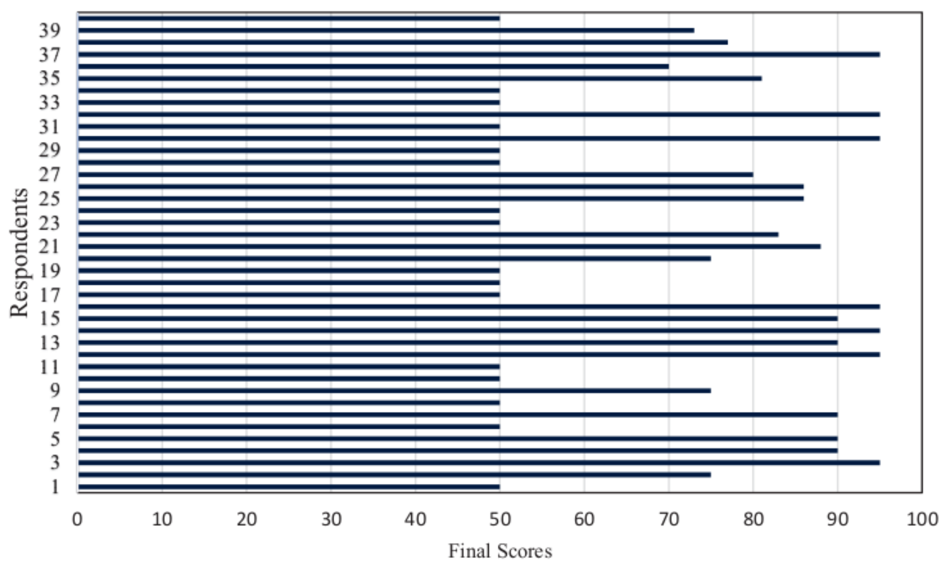

FIGURE 4. Scores for testing the effectiveness of the laboratory work module.

The last step of the research is to communicate those results. At the stage of communicating the test results of the laboratory work module, the product has been produced. The results of the evaluation or analysis of data obtained regarding the laboratory work module that was developed to test the effectiveness of lawsone and its derivatives as a sensitizer in dye-sensitized solar cells which aims to determine the validity, practicality, and effectiveness of the modules that have been made have met the criteria of being very valid and very practical and effective to use. The communication process of the results of this data analysis contains various information about the process of product design and development, the contribution of products developed in research to the realm of education, the relationship between research conducted with previous studies, and how the suitability of the results of data analysis with the objectives of the research carried out previously set.

CONCLUSION

A laboratory work module based on computational chemistry tests the effectiveness of lawsone and its derivatives as a sensitizer in dye-sensitized solar cells has been developed. Parameters of validity, practicality, and effectiveness are in the highly valid, practical, and effective category for laboratory work in computational chemistry courses. This module will be implemented in computational chemistry courses in the 2022/2023 academic year.

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PAGE 1

PAGE 2

PAGE 3

PAGE 4

PAGE 5

PAGE 6

PAGE 7

PAGE 8