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Development of Learning Media Based on Computation Method in Molecular Shape

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ABSTRACT
Good learning media are needed to improve the quality of learning. One of the media that can be used is the use of computer technology, one form of application of computer technology in chemistry is computational chemistry. This study aims to determine the assessment of expert teams on computational method based learning media on Molecular Shape material based on BSNP and find out whether there is a difference in the improvement of student learning outcomes taught with Computational Method Based Learning media on molecular shape material using NWChem software and students taught with using Chemsketch software. This type of research used is research and development that is modified from the development of the ADDIE model (Analysis, Design, Development, Implementation, and Evaluation). The data sources in this study were 3 expert validators and chemistry students at Medan State University totaling 44 students using a purposive sampling data collection technique. The results showed that the assessment of the expert team on computational learning media based on the Molecular Shape material based on BSNP on the aspect of content worthiness had an average percentage value of 96%, 97% language worthiness, and 85% presentation feasibility analysis and it was concluded that the media was very feasible for used and does not need to be revised. Furthermore, there is a difference in the improvement of student learning outcomes taught by the Computational Method Based Learning media on molecular shape material using NWChem software and students who are taught using Chemsketch software.

Keywords: *NWChem, computational chemistry, molecular shape, learning outcomes*

1. INTRODUCTION

Chemistry is built by three levels of representation, namely the macroscopic, microscopic and symbolic levels [1]. To develop students' understanding of chemistry, learning must guide them using various representations and linking these three levels of representation so that students can obtain the full chemical concept.

Chemistry contains many abstract concepts so understanding them requires imagination with the help of images or visuals. The inability of students to understand chemical concepts will lead to wider problems in learning the concepts of chemistry in general, which in turn can give the impression that chemistry is a science that is difficult to understand [2].

Stated that chemistry is a very complex subject, students' misconceptions are not only due to chemical complexity but because of the way the concepts are taught [3]. These problems can be overcome by the presence of innovations that can be used to make learning more effective and involve student activity, which can be in the form of learning media assistance [4].

Good learning media are also needed in improving the quality of learning. The development of appropriate knowledge in the field of information and communication technology is the optimal use of computers in learning activities. One of the media that can be used is the use of computer technology, computer media such as Lectora Inspire which is taught using power point media to get good and effective results as a learning tool to support student learning activities [5]. One form of application of computer technology in chemistry is computational chemistry. Computational chemistry is the application of quantum mechanical theory in determining the properties of atoms and molecules. The advantage of computational chemistry is the result of quantum mechanics

calculations that can be visualized so that it can be used as a learning medium. Besides being able to visualize it, computation can also create animated motion of particles according to vibrational motion. Computational chemistry can be used as a medium in describing molecular shape modeling. Through molecular modeling, students are able to better visualize three-dimensional structures and can improve student understanding [6-8].

Teaching and learning topics in chemistry related to chemical bonds can be enhanced by using computer-assisted teaching materials [9]. Now that computational chemistry is advancing and developing [10], rapid advances in hardware and software can drive computational chemistry to become a strategic tool for productivity for chemists [11].

Computational chemistry methods are very flexible and almost all material chemistry practices both simple and with a high degree of difficulty can be modeled well using computational chemistry in several softwares including NwChem, Hyperchem, and Chemsketch [12]. Another advantage of using computational chemistry modeling is that it is inexpensive, has a high degree of accuracy, shortens practice time, is harmless and can certainly help improve understanding of chemical matter optimally [13] and can be used to gain a deeper understanding of experimental chemistry [14].

Through individual experience with computational modeling, students get a more complete and correct understanding of structure, bonding, and reactivity [15]. In addition, the use of teaching chemical bonds through animation can improve academic achievement and correct understanding of the nature of particulate matter [16].

Animation and visualization programs in computational chemistry can use Jmol, Marvin Sketch, Chemdraw and Avogadro software, in these applications the material of molecular shapes in chemical bonds can be clearly visualized. Activities that integrate visualization tools with active and cooperative learning strategies can build students' knowledge about the concept of chemical bonds [17].

NWChem is a software package for computational chemistry on massive parallel computing systems developed by the high-performance computing chemistry group for environmental molecular science laboratories [18]. NWChem is an ab initio computational chemical software package that provides many methods for calculating the properties of molecular and periodic systems using standard quantum mechanical descriptions of functions or electronic wave densities [19].

The most basic thing from this research is that computers cannot only function as word processing or simple calculation processors. Nowadays computer technology is used in explaining the properties of atoms or molecules through computational chemical calculations. In 1998 John Anthony Pople (Burnham on Sea, 31 October 1925 - 15 March 2004) a theoretical chemist won the Nobel Prize in Chemistry for his development of computational methods in quantum chemistry [20].

In addition to being easy to install, NWChem has other advantages that it has full features [4]. In addition, NWChem can predict the structure, reactivity, and reaction mechanism and can determine the transition state and the activation energy / inhibition of organic reactions.

2. METHOD

This study uses the ADDIE development model (Analysis, Design, Development, Implementation, Evaluation). Research has been conducted at Medan State University (Unimed), Jalan Willem IskandarPasar V, Medan 20221, North Sumatra. The study was conducted in February to May 2020.

The population in this study were all 6th semester students studying chemistry bonding courses. Chemistry education students in 2017 class B and C with each student winning 22 people using purposive sampling data collection techniques.

Research instruments in the form of questionnaires based on BSNP, valid and reliable objective tests and student perception questionnaires. The data analysis technique used is the two-party T-test (Independent Sample T-Test) which has a normal and homogeneous distribution system.

3. RESULT AND DISCUSSION

In this study begins with the analysis stage, namely by analyzing the needs, analysis of teaching materials, and analysis of learning media. In this needs analysis, it refers to the curriculum of the Indonesian National Qualification Framework (KKNI) in the Department of Chemistry, Chemistry Study Program, FMIPA UNIMED, which can be seen in table I.

In the curriculum listed learning outcomes courses and sub achievement learning chemistry courses for molecular shape material. From the CPMK and Sub CPMK, indicators are taken in developing learning media. States that competency development using computational methods can increase the depth and complexity of the laboratory curriculum [21].

Table 1. Requirements Analysis

Requirements Analysis	Analysis Results
Course Learning Achievement	Mastering theoretical concepts about the structure, dynamics and energy of chemicals and the basic principles of separation, analysis, synthesis and characterization.
Sub Learning Subjects	Being able to analyze the concept map and understand each material related to ionic bonds, covalent bonds, Molecular Forms, Bonds between Mocellulos and Molecular Orbital Theory.
Indicators in the development of instructional media	1) Identify and analyze molecular shape characteristics based on VSEPR theory 2) Develop the idea of making media to show or simulate various molecular shapes. 3) Identify and analyze molecular shape characteristics based on the concept of hybridization.

Then in the analysis of instructional materials the researchers conducted interviews and found that in the chemical bonding course there was no special book that became a manual or handbook for students while attending the chemical bonding course. And in the analysis phase of the learning media used the researchers also conducted interviews with students and it can be seen that during the learning process the lecturer who teaches chemical bonding courses uses powerpoint media, and the molecular shapes used on the media are still derived from the images located on books and the internet, and molecular shapes don't yet have animation. In order for the media to be developed according to the needs in the field, a study / analysis of the needs of the media program needs to be carried out [22]. Other studies further state that integrating various media into learning is very important to improve student learning outcomes and improve the teaching skills of the teacher itself [23-24].

Next, the design stage is carried out, the learning media developed are using the NWChem application in computational calculations, then the results of the computational calculations are visualized using Jmol and taught using Powerpoint. Powerpoint was chosen because the application has complete features and is available on every computer so that it can be used by anyone, anytime and anywhere.

The next stage is a standardization assessment of the development of instructional media based on computational methods on Molecular Form material based on BSNP. After the developed media is finished, validation is carried out to the expert validator. The average results of the percentage validation can be seen in Figure 1 so it can be concluded that the media is very feasible to use and does not need to be revised. This is in line which shows that computer-based learning media is very suitable for chemistry learning [25].

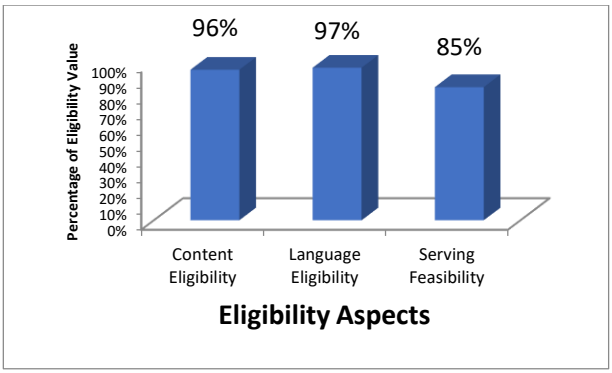

Figure 1. Graphic Results of Feasibility Analysis Learning Media Based on Computational Methods in Molecular Material Material

States that activities that integrate visualization tools with active and cooperative learning strategies can build students' knowledge about the concept of chemical bonds [17]. Furthermore the use of interactive animation has a positive effect on student understanding [26].

Then in this study also seen differences in the increase in student learning outcomes taught by Computational Method Based Learning media on molecular shape material using NWChem software (Experiment 1) and students who were taught using Chemsketch software (Experiment 2). From the results of the implementation of the experimental class 1 and experimental class 2 has an average value of learning outcomes as in table II and has a percentage increase in learning outcomes of 71.43% and 56.30% which can be seen in table III.

Table 2. Pretest and Posttest Data

Data	Experiment Class 1			Experiment Class 2		
	Lowest score	**Highest Scores**	**Average**	**Lowest score**	**Highest Scores**	**Average**
Pretest	50	80	67,73	40	90	68,86
Posttest	70	100	89,55	70	100	84,77

Table 3. Percentage Increase In Learning Outcomes

Descriptives

	Kelas			Statistic	Std. Error
N_Gain	Eksperimen 1	Mean		.7143	.05266
		95% Confidence Interval for Mean	Lower Bound	.6048	
			Upper Bound	.8239	
		5% Trimmed Mean		.7194	
		Median		.6667	
		Variance		.061	
		Std. Deviation		.24700	
		Minimum		.33	
		Maximum		1.00	
		Range		.67	
		Interquartile Range		.57	
		Skewness		-.121	.491
		Kurtosis		-1.515	.953
	Eksperimen 2	Mean		.5630	.05146
		95% Confidence Interval for Mean	Lower Bound	.4560	
			Upper Bound	.6700	
		5% Trimmed Mean		.5586	
		Median		.5857	
		Variance		.058	
		Std. Deviation		.24139	
		Minimum		.20	
		Maximum		1.00	
		Range		.80	
		Interquartile Range		.33	
		Skewness		.414	.491
		Kurtosis		-.511	.953

Of the two classes that obtained the average improvement in student learning outcomes the best was the experimental class (71.43%). This shows that NWChem learning media can improve student learning outcomes because in this media students can learn molecular shape material with pictures and animated videos of molecular shapes. This is consistent with research showing that learning media developed can improve learning outcomes in molecular shaped material [27].

Other research states that the use of Chemsketch media in learning can improve learning outcomes in the classroom [28]. The use of technology media in learning can also increase students' scientific knowledge from pretest to posttest and students are motivated and enjoy the experience [29].

In this study there are also differences in student learning outcomes with the two learning media which can be seen in table IV where the Sig (0.046) is smaller than 0.05. So it can be seen that there are differences in the increase in student learning outcomes taught by instructional media based on computational methods in molecular shape material using NWChem software and students taught by using Chemsketch software. In the use of computational chemistry can improve student understanding better, in describing molecular modeling that can be easily used to improve student understanding [6].

Table 3. Percentage Increase In Learning Outcomes

Nilai N-gain	Sig	α	Keterangan
Equal variances asuumed	0,046	0,05	Ha diterima

4. CONCLUSION

The results of the needs analysis are obtained by learning indicators of learning achievements and sub achievement of chemical bonding courses in the development of instructional media, from the analysis of instructional materials and instructional media information is obtained that there is no specific book used as a guidebook and the media used are powerpoint media, where the pictures are pictures on these media come from books and the internet, and molecular shapes don't yet have animation.

The results of the standardization of the development of instructional media based on computational methods on the material Molecular Shape based on BSNP conducted by expert validators obtained a percentage of content worthiness of 96% (very feasible and does not need revision); percentage of language worthiness of 97% (very feasible, and does not need to be revised); and percentage of presentation eligibility of 85% (very feasible and does not need to be revised).

There are differences in student learning outcomes with the two learning media where the value of Sig (0.046) is smaller than 0.05. So it can be seen that there are differences in the increase in student learning outcomes taught by the media of Computational Method Based Learning on molecular shape material using NWChem software and students who are taught using the Chemsketch software.

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