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Original Research Article

The need analysis for computational chemistry based learning media atomic structure and chemical bonding basic chemistry courses

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ABSTRACT

The aim of this research is to analyze students' needs for computational chemistry-based learning media on atomic structure and chemical bonding in the Basic Chemistry course. The population of this study were the first grade students of the Chemistry Department, FMIPA Unimed. The number of samples in this study was 93 students from three classes. The instruments used are multiple choice questions and questionnaires to determine mastery of atomic structure and chemical bonding. The research results show that the average score is 34.430 (poor category). The average score achieved in atomic structure material was 33.16 (very poor). The lowest score achieved in the atomic properties sub-material was 9.3. The average score achieved in chemical bonding material was 36.1 (very poor). The lowest score achieved in the properties of ionic compound sub-material was 17.5. The results of the questionnaire showed that the atomic structure material that students considered the most difficult was the wave mechanics atomic model at 72.233 (quite difficult), while for chemical bonding material it was the octet and duplet rule at 71.055 (quite difficult).

Introduction

The Basic Chemistry course is one of the basic courses for students in the Chemistry Department. This course is a basic course which aims to equip students with various basic concepts within the scope of chemistry. Good mastery of basic chemistry material will make it easier for students to study various chemical materials at a higher level. The characteristic of the structure atom and chemical bond are very abstract so that we cannot see with the naked eye various events involving the atomic structure or the process of forming chemical bonds.

In general, chemistry learning activities are built on three levels of representation, namely macroscopic, microscopic and symbolic levels (Treagust et al., 2003). To develop students' understanding of chemical material, the learning activities carried out must use various representations and link the three levels of representation so that students can obtain complete chemical concepts. Presenting chemical concepts in three levels of representation simultaneously is an important aspect that needs to be considered in chemistry learning activities. The tendency is that chemistry learning activities are generally limited to the macroscopic level, microscopic and symbolic representations tend to be ignored. This can cause students tend to have difficulty understanding abstract chemical concepts, which can give rise to misconceptions (Marfali, 2019). Kolomuc & Tekin (2011) stated that chemistry is a very complex subject, student misunderstandings are not only due to the complexity of chemistry but because of the way the concepts are taught.

Spatial ability is an important factor that can influence success in the fields of mathematics and geometry, engineering, chemistry, physics, geology, architecture, health, medicine and dentistry (Lubinski, 2010). Science, mathematics, and engineering are some of the fields where spatial abilities receive the greatest emphasis for success. Likewise, spatial abilities play an important role in student achievement in Science, Technology, Engineering, and Mathematics (STEM) education, which is an innovative teaching approach (Stieff & Uttal, 2015). Bongers et al. (2020) have conducted research on the influence of static and animated representations, initial abilities and spatial abilities on the topic of reaction mechanisms. The results showed that there was no significant difference between static and animated learning conditions. Spatial ability correlates with test accuracy and influences learning outcomes in both conditions.

Study of the influence of computer-assisted 3D modeling learning activities on teachers' spatial abilities and attitudes. Research results show that computer-assisted 3D modeling activities improve teachers' spatial abilities and also improve their attitudes towards 3D modeling (Benzer & Yilzid, 2019). Study of the effectiveness of the program providing spatial visualization treatment to improve students' spatial reasoning and mathematics performance. The research results show that the spatial reasoning enrichment program implemented by teachers can improve spatial reasoning and mathematics performance (Lowrie et al., 2019). Studies reviewing simulations from a research perspective suggest four learning effects help clarify the positive and negative aspects of current simulation designs: image prominence, observation, structuring, and tuning (Lindgren & Schwartz, 2009). Studies related to the ability to handle and learn using visualization have obtained research results showing that understanding visual models is a key factor for students to be successful in learning chemistry (Dickmann et al., 2019).

The results of research on the use of Augmented Reality mobile applications in studying 3-dimensional molecular structures show that the approach using 3D visualization has proven to be relatively well received by students (Aw et al., 2020). The application of computer-based learning activities has been implemented at various levels of education. The advantage of computer-based learning activities is that they can display chemical structures in three dimensions. The process can be applied to create a 3D representation of some 2D object, and the application is useful for visualizing simple stereochemistry, when presenting 3D structures on poster presentations, or in audio-visual presentations (Eriksen et al., 2020). Other research seeks to visualize the molecular conformation and structure of complex compounds as well as chemical transformations in 3D to help students understand molecular structure and chemical reaction mechanisms at the molecular level. A comprehensive survey was conducted to collect student feedback on the effectiveness of this media and student perceptions of course material using this technology (Abdinejad et al., 2020).

Molecular modeling studies have been carried out chemical research activities. Study of the interactions between β-carotene molecules and various solvents. The results obtained were that the mixture of β-carotene-ethanol and β-carotene-methanol had the best interaction (Nugraha et al, 2021). Determination of the polymeric structure of the complex compound iron(II) 1,2,4 H-triazole. The results obtained are data on the Fe-N bond length, the distance between the Fe(II) ion and other Fe(II), and the dihedral angle (Nugraha et al., 2019). Determination of spin transition properties in iron(II) 1,2,4 H-triazole complex compounds. The research results obtained data on the length of the Fe-N bond, the distance between the Fe(II) ion and other Fe(II), and the dihedral angle in the low spin state and the high spin state. In addition, transition temperature data and spin transition curve data were obtained (Nugraha et al., 2022).

Methods

Population and Sample

The population in this study was the first grade students of the Chemistry Department, FMIPA, Medan State University who took the Basic Chemistry course. Sample selection was carried out randomly with the assumption that the abilities of the students in each class were relatively the same. The total sample in this study was 93 students consisting of 3 classes, namely: Chemistry Education Study Program, namely: Program Studi Pendidikan Kimia (PSPK) 2023B and PSPK 2023C classes and Chemistry Study Program, namely: Program Studi Kimia (PSKM) 2023B class.

Research Instrument

The instrument used to analyze the need for computational chemistry-based learning media on atomic structure and chemical bonding in the Basic Chemistry course is a test in the form of multiple choices and a questionnaire with a Likert scale. The test is used to determine the level of student understanding of concepts on the subject of atomic structure and chemical bonds. The number of questions for atomic structure and chemical bonding is 25 each. The cognitive level of the test questions is distributed at cognitive levels C3, C4, and C5.

The questionnaire used to explore students' perceptions of atomic structure and chemical bonding material used a Likert scale (Boone & Boone, 2012; Willits et. al., 2016) with five answer options. The questions given to students related to students' difficulties with the sub-material of atomic structure and chemical bonds. The sub-material in this questionnaire has several similarities with the sub-material presented in the test questions.

Results and Discussion

Determining the level of difficulty of students majoring in chemistry at FMIPA Unimed in atomic structure and chemical bonding was carried out using test instruments and questionnaires. The results obtained from test data are students' ability to understand the concepts of atomic structure and chemical bonds. These data provide an overview of the understanding of Chemistry Department students in the second semester of the 2023/2024 academic year. The average value of the material on atomic structure and chemical bonds of the PSPK 2023B, PSPK 2023C and PSKM 2023B classes is shown in Fig-1.

A more in-depth analysis of the average value can be done by looking at the achieved value for each sub-material for atomic structure and chemical bonds. Data on the average achievement scores for each sub-material in the atomic structure material are presented in Table 1.

The atomic structure material is material that makes a major contribution to the concepts of chemical bonding. As a result of this relationship, mastery of atomic structure material will contribute to the understanding of chemical bonding material. If mastery of atomic structure material is good enough, it is hoped that it will make a positive contribution to mastery of chemical bonding material and vice versa. Data on the average achievement scores for each sub-material in the chemical bond material are presented in Table 2.

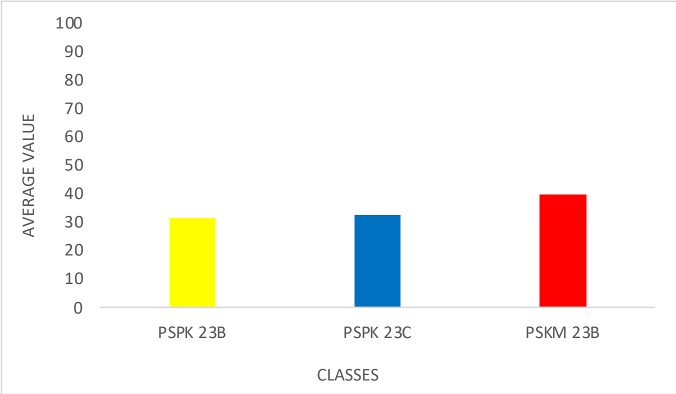

Fig-1. Average material values for atomic structure and chemical bonds.

A study of the level of difficulty of Chemistry Department students regarding atomic structure and chemical bonds was also carried out using a questionnaire. The use of questionnaires in determining students' level of difficulty is to complete the data obtained from tests given to students. Data on the level of difficulty of Chemistry Department students for PSPK 2023B, PSPK 2023C, and PSKM 2023B classes in atomic structure material is presented in Table 3. Data on the level of difficulty of Chemistry Department students for PSPK 2023B, PSPK 2023C, and PSKM 2023B classes in the chemical bonding material are presented in Table 4.

Table 1. Average achievement scores for each sub-material in atomic structure material

No	Field of Study	Average value
1	Development of atomic theory	28.1
2	The basic particles that make up atoms	41.7
3	Dalton's atomic model	25
4	Thomson's atomic model	73.3
5	Rutherford's atomic model	39
6	Bohr's atomic model	24.5
7	Wave mechanics atomic model	31.3
8	Electron configuration in an atom	33.9
9	Quantum numbers	25.5
10	Atomic properties	9.3
	Avarage	33.16

Table 2. Average achievement scores for each sub-material in the chemical bond material

No	Field of Study	Average value
1	The concept of stability in the formation of chemical bonds	34.2
2	Octet and duplet rules for the formation of chemical bonds	31.6
3	The process of forming ionic bonds	28.9
4	Properties of ionic compounds	17.5
5	The process of forming covalent bonds	54.4
6	Distinguish between ionic bonds and covalent bonds	38.6
7	Properties of covalent compounds	51.3
8	Distinguish between polar covalent bonds and non-polar covalent bonds	27.2
9	Bond length, bond energy, and bond order	27.2
10	Resonance structure	49.1
11	Electron domain theory to determine molecular structure	34.3
12	Exceptions to the octet rule in covalent bond formation	21.9
13	Molecular shape	34
14	Hybridization	29.8
15	Intermolecular forces	44.7
16	Hydrogen Bonding	52.6
	Total Average value	36.1

The average score for PSPK 2023B, PSPK 2023C, and PSKM 2023B classes for atomic structure and chemical bonding from the Figure 1 respectively is 31.471; 32,667; and 39.724, while the average score for the three classes was 34.430 (poor category). These data show that the average score for the PSKM 2023B class is the highest, followed by the PSPK 2023C class and the lowest is the average score for the PSPK 2023B class. The average score achieved for the three classes is in the very low category, so it can be stated that students' understanding of atomic structure and chemical bonds is very low. If we look at the scores achieved by individual students, the results show that there were no students who got a score greater than 60.

The average score achieved in atomic structure material from the Tabel 1 was 33.16, this data can be categorized as very poor. The lowest score achieved in the atomic properties sub-material was 9.3 and the highest score in the Thomson's atomic model sub-material was 73.3. Achievements in other sub-materials range between 24.5 for the Bohr's atomic model sub-material up to 41.7 for the basic particles that make up the atoms sub-material. These data show that the textbooks and media that will be developed must provide reinforcement for mastery of these sub-materials.

Table 3. Student difficulty level in atomic structure material.

No	Statement	Questionnaire results			Average
		PSPK 2023B	PSPK 2023C	PSKM 2023B	
1	Difficulty learning the subject of atomic structure	68.824	70.968	65.625	68.472
2	Difficulty understanding the development of atomic theory	73.529	65.161	67.500	68.730
3	Difficulty in understanding the basic particles that make up atoms	65.882	66.452	63.750	65.361
4	Difficulty understanding electron particles	62.941	64.516	64.375	63.944
5	Difficulty understanding proton particles	62.353	63.871	57.500	61.241
6	Difficulty understanding neutron particles	63.529	64.516	60.000	62.682
7	Not aware of the existence of particles other than electrons, protons and neutrons	73.529	67.097	63.750	68.125
8	Difficulty understanding Dalton's atomic model	65.294	67.097	61.250	64.547
9	Difficulty understanding Thomson's atomic model	68.235	70.323	66.875	68.478
10	Difficulty understanding Rutherford's atomic model	71.765	70.323	68.125	70.071
11	Difficulty understanding Bohr's atomic model	69.412	67.097	63.125	66.545
12	Difficulty understanding the atomic model of wave mechanics	77.647	69.677	69.375	72.233
13	Difficulty understanding the configuration of electrons in atoms	60.000	57.419	56.250	57.890
14	Difficulty understanding the four quantum numbers	74.118	65.806	63.750	67.891
	Avarage	68.361	66.452	63.661	66.158

The average score achieved in chemical bonding from the Tabel 2 is 36.1, this figure can be categorized as very poor. The lowest score achieved in the Properties of ionic compound sub-material was 17.5 and the highest score in the The process of forming covalent bonds sub-material was 54.4. The achievements in other sub-materials were more evenly distributed, ranging between 21.9 for the Exceptions to the octet rule in covalent bond formation sub-material up to 52.6 for the Hydrogen Bonding sub-material. These data show that the textbooks and media that will be developed must provide reinforcement for mastery of these sub-materials.

Based on the data presented in Table 3, it shows that the average level of difficulty of atomic structure material is 66,158 (quite difficult). This data shows a level of difficulty that is almost the same as the quite difficult category with varying average values for the three classes observed. The material considered the most difficult by students is the wave mechanics atomic model (72.233), Rutherford's atomic model (70.071), and the development of atomic theory (68.730). The material considered easiest by students is the configuration of electrons in atoms (57,890), proton particles (61,241), and neutron particles (62,682). In general, the data from this questionnaire shows that students find the atomic structure material quite difficult. This data is slightly different from the test result data which shows that the average value for atomic structure material is 33.16 (very poor category).

Table 4. Student difficulty level in chemical bonding material.

No	Statement	Questionnaire results			Average
		PSPK 2023B	PSPK 2023C	PSKM 2023B	
1	Difficulty learning the subject of chemical bonds	60.588	63.226	60.000	61.271
2	Difficulty understanding the concept of stability in the formation of chemical bonds	72.353	65.806	66.875	68.345
3	Difficulty understanding the octet and duplet rules in the formation of chemical bonds	73.529	68.387	71.250	71.055
4	Difficulty understanding electron particles	62.941	64.516	64.375	63.944
5	Difficulty understanding the process of ionic bond formation	64.118	63.226	63.750	63.698
6	Difficulty understanding the properties of ionic compounds	59.412	63.226	60.625	61.088
7	Difficulty understanding the process of covalent bond formation	64.118	62.581	63.750	63.483
8	Difficulty understanding Dalton's atomic model	65.294	67.097	61.250	64.547
9	Difficulty distinguishing between ionic bonds and covalent bonds	64.118	60.000	55.625	59.914
10	Difficulty distinguishing between polar covalent bonds and non-polar covalent bonds	70.588	67.097	60.000	65.895
	Avarage	67.353	65.420	63.813	65.528

Based on the data presented in Table 4, it shows that the average level of difficulty of chemical bonding material is 65,528 (quite difficult). This data shows a level of difficulty that is almost the same as the quite difficult category with varying average values for the three classes observed. The material considered the most difficult by students is the octet and duplet rule for the formation of chemical bonds (71.055), the exception to the octet rule for the formation of covalent bonds (70.696), and electron domain theory for determining molecular structure (69.838). The material that students consider the easiest is differentiating between ionic bonds and covalent bonds (59.914) and understanding the properties of ionic compounds (61.088). In general, the data from this questionnaire shows that students find chemical bonding material quite difficult. This data is slightly different from the test result data which shows that the average value of atomic structure material is 36.1 (very poor category).

Based on quantitative data obtained from test results and data obtained from questionnaires, it shows that most of the material on atomic structure and chemical bonds is not mastered by students. Questionnaire data shows that students feel they have quite a lot of difficulty in understanding concepts in atomic structure and chemical bonds. Apart from that, based on the study of the RPS that has been developed, there are several sub-materials that must be added to these two materials. The sub-material that needs to be added to the atomic structure material is the basic particles that make up atoms (electrons, protons and neutrons), additional discussion of the Thomson and Bohr atomic model, while for the chemical bond material is the process of forming ionic and covalent bonds, electron domain theory, and exceptions to the octet rule.

Strengthening mastery of the sub-material of the basic particles that make up atoms (electrons, protons, and neutrons) can be done through presenting experiments in the discovery of these particles. Strengthening the sub-material of Dalton, Thomson, Rutherford, and Bohr's atomic models can be done by presenting visual models of the atomic model. Strengthening the understanding of the differences between ionic and covalent bonds can be done by simulating the vibrational movements of compounds that have both chemical bonds. Strengthening the understanding of the differences between polar and non-polar covalent bonds can be done by presenting contour images of the electron density of each -each of these compounds. Understanding molecular shapes that comply with the octet rule and those that deviate from the octet rule can be done by presenting the molecular shapes.

Based on data from research regarding analysis of the need for computational chemistry-based learning media, it shows that learning about atomic structure and chemical bonds will be more effective if you use media with pictures of chemical structures and animations. The use of animation in chemistry learning can improve students' spatial abilities. The use of animation in learning reaction mechanism material can improve students' spatial abilities (Bongers et al., 2020). Understanding visual models is a key factor for students to succeed in chemistry learning activities, and visual models act as mediators to connect prior knowledge and content knowledge in chemistry studies (Dickmann et al., 2019). Chemical studies using 2D and 3D molecular structures can improve students' understanding of the simple stereochemical material (Eriksen et al., 2020).

Conclusion

The research results show that the average score for the PSPK 2023B, PSPK 2023C, and PSKM 2023B classes respectively is 31.471; 32.667; and 39.724, while the average score for the three classes was 34.430 (poor category). The average score achieved in atomic structure material was 33.16, this data can be categorized as very poor. The lowest score achieved in the Atomic properties sub-material was 9.3 and the highest score in the Thomson's atomic model sub-material was 73.3. The average score achieved in chemical bonding is 36.1, this data can be categorized as very poor. The lowest score achieved in the Properties of ionic compound sub-material was 17.5 and the highest score in the The process of forming covalent bonds sub-material was 54.4. The learning of atomic structure and chemical bonds will be more effective if you use media with pictures of chemical structures and animations.

Conflict of Interests

The author(s) declares that there is no conflict of interest in this research and manuscript.

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