# Development of Learning Media Based on Visualization of Computation Chemical Calculation Results

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**Abstract.** This study aims to determine the feasibility of learning media for electrolyte and non-electrolyte solutions based on visualization of computational chemical calculations. This type of research is development research that refers to the ADDIE model. This study uses a modified BSNP validation sheet which is validated by four validators: two chemistry teachers, material experts, and two media expert lecturers. The results of the needs analysis are the results of validating the feasibility of learning media based on visualization of computational chemistry calculations on electrolyte and non-electrolyte solution materials found on BSNP obtained an average percentage of content eligibility is 95%, language feasibility is 96%, and presentation feasibility is 94%. From the average percentage value of the three aspects, it is obtained 95%, meaning that the media is very feasible to use. The percentage of student responses to learning media is 87.97%.

Keywords: learning media, visualization, computing

### **1** Introduction

In the 2013 curriculum, improving the quality of learning cannot be separated from the learning process. The learning process is one element of the standard procedure that changes to achieve learning success and the formation of student competencies [1]. The method of learning chemistry in schools is still a problem that needs to be solved. Most chemistry teachers still use conventional and less innovative ways of teaching chemistry so that students feel uninterested in studying chemistry and even think that chemistry lessons are complex [2].

Teachers must be able to provide or apply appropriate learning media in chemistry learning [3]. Chemistry learning media dramatically affects student learning outcomes [4]. Learning media will make it easier for teachers to explain difficult-level material to be easier to understand [5]. With media application in chemistry learning, learning is made interesting with animation, sound, and images [6]. The use of interactive media is very influential on

student learning outcomes [7]. Utilizing technological developments in teaching and learning activities with computers has an excellent opportunity for students and teachers to combine active learning with computer technology [8]. The use of computer-based media has a different way to help students' problems in learning chemistry than media without computers [9].

Currently, developments that are by knowledge in the field of information and communication technology are the optimal use of computers in learning activities. Good learning media is also needed to improve the quality of learning. One of the media that can be used is PowerPoint, which is equipped with chemical structures and animations. The system and vibrancy of the chemical structure were developed using computational chemical calculations. The media produced is the application of computational chemistry calculations in the field of teaching chemistry [10].

Computational chemistry methods are very flexible. Almost all practical chemistry materials, both simple and high difficulty levels, can be well modeled using computational chemistry in software, including NwChem, Hyperchem, and Chemsketch [11]. The use of computational chemistry modeling has the advantage that it is inexpensive, has a high level of accuracy, shortens practice time, is not dangerous, and helps improve understanding of chemistry optimally [12]. Many applications of computational chemistry can be used to enhance students' experience of chemical structures and bonds. An ab initio computational chemistry software package that provides multiple methods for calculating the properties of molecular and periodic systems using standard quantum mechanical descriptions of the electronic wave function or density [13].

Visualization programs in computational chemistry can use Jmol, Chemdraw, and Avogadro software. In these applications, chemical bonding materials can be visualized in real terms. Avogadro is software that can be used to create 3-dimensional molecular shapes. Visualization using Avogadro software can explain understanding abstract concepts to be more concrete, easily captured by students, and fun to follow [14]. Avogadro software can bring students closer to molecules, reveal microscopic details, and help them understand chemical properties, chemical reactions, and other chemical phenomena [15].

Computational chemistry calculation methods can determine the energy and intermolecular distances in organic solution materials. The compound with the lowest power is the most stable compared to the mix with the highest point [16]. The benefits of computational chemistry calculations from the visualization results using Jmol software can produce thermodynamic data of compounds and the structure of interactions between compounds [17]. Computational chemical analyses and visualization using Jmol and Avogadro can determine the structure and stability of polymer complexes, the distance between ions, bond lengths, and the energy of complex formation with ligands [18].

# 2 Method

This research is research and development (Research and Development). The development research method applied in this research is the ADDIE development model starting from Analysis (Analysis), Design (Design), and Development (Development).

The analysis phase is carried out to analyze the needs needed to help students overcome learning difficulties in electrolyte and non-electrolyte solutions related to chemical structures. The data obtained are used to determine the need for the media developed in this study in the form of learning media for electrolyte and non-electrolyte solutions based on visualization of computational chemical calculations.

In the design phase, the researcher prepares the initial product or product design. At this stage, the activities carried out are designing learning media, determining compounds, developing research instruments consisting of the development stage carried out (1) making the structure of the compound with NWChem, namely the structure of the compound NaCl, HCl, NaOH, HF, H<sub>2</sub>S, NH<sub>3</sub>, H<sub>2</sub>O, CH<sub>3</sub>OH, C<sub>2</sub>H<sub>5</sub>OH, and C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>; (2) visualization and animation of compounds with Avogadro and Jmol; (3) media creation on PowerPoint; (4) validation of learning media to two media expert lecturers and teaching materials to two chemistry teachers; (5) improvement of learning media and teaching materials; (7) the final product of learning media. The expert validation assessment sheet criteria are based on the BSNP, which has been modified using a Likert scale.

# **3 Results and Discussion**

The results of the calculations using the NWChem version 6.6 software to obtain the calculated data using the Unrestricted Hartree-Fock (UHF) method with a base set of 3-21G. The results of the calculation of NaCl, HCl, and NaOH compounds which are vital electrolytes using NWChem software, are then visualized using Jmol software in 3 Dimensional (3D) form as presented in the Figure below:



Figure 1. The structure of the visualization NaCl



Figure 2. The structure of the visualization HCl



Figure 3. The structure of the visualization NaOH

The calculation results of HF,  $H_2S$ ,  $NH_3$ , and  $H_2O$  compounds, weak electrolyte solutions using NWChem software, are then visualized using Jmol software in the form of 3 Dimensions (3D) presented in the Figure below.



Figure 4. The structure of the visualization HF



Figure 5. The structure of the visualization H<sub>2</sub>S



Figure 6. The structure of the visualization NH<sub>3</sub>



Figure 7. The structure of the visualization H<sub>2</sub>O

The result of compound calculation  $CH_3OH$ ,  $C_2H_5OH$ , and  $C_6H_{12}O_6$  which is a non-electrolyte solution using NWChem software, then visualized using Jmol software in the form of 3 Dimensions (3D) which can be seen in the Figure below.



Figure 8. The structure of the visualization CH<sub>3</sub>OH



Figure 9. The structure of the visualization C<sub>2</sub>H<sub>5</sub>OH



Figure 10. The structure of the visualization  $C_6H_{12}O_6$ 

The process of making learning media into products in the form of 3D visualization media and animations on electrolyte and non-electrolyte solution materials in the form of powerpoints. The following is an example display of the learning media products that have been made.



Figure 11. Display of the Media Home

The initial media display includes indicators, objectives, materials, summaries, and evaluations.



Figure 12. Display Indicator

Indicators are things to be achieved in the learning process on this media.



Figure 13. Display of learning objectives

Learning objectives contain the goals to be achieved in this media.



Figure 14. Display Material Menu

The material in this media about electrolyte and non-electrolyte solutions is equipped with visualization of computational calculations and animations of their compounds.



Figure 15. Summary Menu

The summary contains the core of the material described in bullet points to make it easier for students to understand the concept of the material.



Figure 16. Evaluation Display

The evaluation, which consists of five description questions, aims to test the extent to which students can understand the concept of the material.

Learning media based on visualization of computational chemistry results has been validated using the modified National Education Standards Agency (BSNP) eligibility standards. The developed media is assessed based on three eligibility standards according to BSNP, namely content feasibility, language feasibility, and presentation feasibility with material expert validators, namely two chemistry teachers and media expert validators, namely two chemistry lecturers.

The feasibility level of the electrolyte and non-electrolyte solution learning media developed based on the BSNP, which includes the feasibility of content, language feasibility, and presentation feasibility, is shown in Figure 17.



Figure 17. Graph of Media Feasibility Analysis Results Based on Visualization of Computational Chemistry Calculation Results on Electrolyte and Non-Electrolyte Solution Materials.

From the picture above, the media analysis results developed based on the BSNP questionnaire obtained an average percentage value of 95% content eligibility, 96% language eligibility, and 94% presentation feasibility, meaning that the media is very feasible and does not need to be revised. From the value of these three aspects, 95% is obtained, meaning that the press is possible to use.

Learning media based on 3D visualization and animation is very feasible/valid to be used for chemistry learning [19]. The results of media validation based on computational chemistry methods obtained an average value of 91% of content eligibility, 88% of language eligibility, and 75% presentation feasibility [10]. The results of the validity of learning media using computational methods obtained a percentage of media eligibility of 90.8% [20]. Compared with the visualization-based media validation results of computational chemistry calculations that have been carried out, it can be said that the percentage of media feasibility is greater than the percentage of media feasibility [10] and [20]. This is due to the different validators, the different chemicals developed, and the use of different animations.

Providing student response questionnaires obtained a percentage of student responses to the media of 87.97%. This means that the learning media for electrolyte and non-electrolyte solutions based on the visualization of computational chemistry results is very feasible to use. Student response to computational-based hydrocarbon media is 92.6% [20]. Student response to the molecular form media based on computational chemistry is 79% [10]. Student response to the media developed based on weblogs was 74.5% [21]. When compared with previous studies, the results of the percentage of student responses to electrolyte and non-electrolyte

solution media based on visualization of computational chemistry calculations are lower than in previous studies, and this is due to differences in student samples, differences in response questionnaires, and differences in the material applied to the media.

### **4** Conclusion

Based on the research conducted, it can be concluded that the results of the validation of the feasibility of learning media based on visualization of computational chemistry calculations on electrolyte and non-electrolyte solution materials based on BSNP obtained an average percentage of 95% content eligibility, 96% language eligibility, and 94% presentation feasibility. From the value of the three aspects obtained, 94% means that the media is very feasible to use. The percentage value of student responses to learning media is 87.97%, which is possible to use.

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