

# Analysis of the Need for Development of Computational Chemistry-Based Learning Media on the Subject of Hydrocarbons

Rara Gustiana<sup>1\*</sup>, Asep Wahyu Nugraha<sup>2</sup>, Nurfajriani<sup>3</sup>

<sup>1,2,3</sup> Postgraduate Chemistry Education, Medan State University, Jalan Williem Iskandar Pasar V Medan Estate, 20221, North Sumatra, Indonesia

\*Correspondence: raragustiana27@gmail.com

## Article History

Received 06 19<sup>th</sup> 2024  
Revised 06 25<sup>th</sup> 2024  
Accepted 06 29<sup>th</sup> 2024  
Available Online 06 30<sup>th</sup> 2024

## Keywords:

*Computational chemistry*  
*Hydrocarbons*  
*Learning media*  
*Needs analysis*

## Abstract

This study aims to analyze the needs before developing computational chemistry-based learning media on hydrocarbon materials. This research is classified as development research developed with the ADDIE model. It's just that the stage used in this study is only limited to the analysis stage. Data collection in research is carried out by literature study methods and field studies with research instruments in the form of questionnaires on learning media needs and interviews by teachers. The location of this study is SMA Negeri Modal Bangsa Arun. Based on the results of interviews with chemistry teachers, it was found that learning hydrocarbon material at the high school level requires more effort because students must understand molecular structure, chemical bonds, and atomic structure. This makes students less understanding of concepts microscopically and can also cause misconceptions. Then, the results of the needs analysis show that there are still limited learning media that support microscopic concepts, especially the shape of molecules in 3-D. Based on the results of this study, it can be concluded that it is necessary to develop computational chemistry-based learning media on hydrocarbon materials.



Copyright: © 2023 by the authors. This is an open-access article distributed under the terms of the Creative Commons Attribution-NonCommercial 4.0 International License. (<https://creativecommons.org/licenses/by-nc/4.0/>)

## 1. Introduction

Chemistry learning includes three aspects of the study that must be understood, namely macroscopic, microscopic, and symbolic aspects. On the macroscopic aspect, teachers often implement it because this level includes real chemical phenomena directly or indirectly in the daily experience of students. Meanwhile, for the microscopic aspect, teachers rarely implement it into learning, because at this level real chemical phenomena are shown at a specific level, so they cannot be seen such as the movement of electrons, molecules, particles, or atoms. Then, for the symbolic aspect, teachers also often implement it because this is related to forms in the form of pictures, calculations and graphs.

One of the chemical substances that is included in the three aspects above is hydrocarbons. Hydrocarbons are one of the chemical materials of high school with basic competencies, namely analyzing the structure and properties of hydrocarbon compounds based on understanding the peculiarities of carbon atoms and their compound classification. In this material, there is also a sub-material on isomerism in alkanes, alkenes, and alkynes.

Based on the results of observations and interviews with chemistry teachers at high school SMA Negeri Modal Bangsa, Arun said that learning hydrocarbon materials at the high school level requires more effort because students must understand molecular structure and naming. This makes students less understanding of concepts microscopically and can also cause misconceptions about chemistry learning. Students also do not understand properly about the structure of existing compounds. This is following the opinion of Setyarini, et al., (2022), that students learn to interpret molecular structures visualized as simple line drawings are difficult to face. In Zuliatin's opinion (2022), chemistry lessons study a substance which includes the composition, structure, properties, changes, dynamics and energetics of substances that involve skills and reasoning. The factors that cause chemistry to be difficult to study are that chemistry requires the ability to think abstractly for study materials, for example, atomic structure, chemical bonds and molecular shapes (Iskandar, 2002).

In addition to abstract and complex chemical materials, it turns out that learning media to improve the quality of learning is still inadequate. The media used is still very limited, teachers only present images of structures obtained from the internet. Then, the textbook used also does not display the 3D structure of hydrocarbon compounds. Thus, students are almost entirely unaware of the 3D shape of structures or molecules. Therefore, this has not been able to increase students' knowledge to be able to visualize molecular structures in three dimensions. The importance of using learning media in addition to increasing students' knowledge can also arouse new desires and interests, arouse learning motivation, and even bring psychological influence on students (Wiratmojo, P & Sasonohardjo, 2002). The use of appropriate learning media is essential when learning because it has various advantages, namely resulting in abstract and complete principles into something clear, simple, and planned (Nurfajriani, Siti, H., & Nur, H., 2020).

The difficulties encountered can be minimized by the use of learning media such as computational chemistry. According to (Paramita et al., 2020), computational chemistry is a branch of chemistry that uses chemical materials that are fed into computer programs to be able to calculate molecular properties (atomic structure, energy and energy difference, charge, dipole moment, reactivity, vibration frequency, and other spectroscopic quantities) and their changes. Computational chemistry can predict the structure, mechanisms and energy of reactions so that users can design the structure and predict the properties of a compound accurately and provide data at the microscopic level (Amalia, Irma., et al.,

2019). The use of software in computational chemistry helps students understand material regarding molecular structure. This is because software in computational chemistry can visualize molecular structures in three dimensions. The use of computational chemistry is a very motivating means to get students involved in chemistry in creating a more realistic and real model of molecular structures (Luciano, E.H., et al., 2014). Some computational chemistry software such as *Jmol*, *Marvin Sketch*, *HyperChem*, *Chemdraw*, *NWChem*, and *Avogadro* can visualize microscopic matter in reality.

Software Avogadro can visualize the shape of the molecule perfectly and include other information about the molecule, one of which is information on the angle of the molecule, the number of masses, atomic numbers, reactivity and so on so that it is very efficient in its use (Nasution, et al., 2023)

Several studies have been conducted on the use of computational chemistry such as the research of Siregar, et al., (2020) using *hyperchem* computing media on molecular materials. The use of *hyperchem* is considered relatively easy and can immediately show the appearance of the structure to be made. The use of *Hyperchem* is suitable for the subject matter of atomic structure, periodic properties, molecular geometry, energy and thermodynamics and chemical laboratories, while for subjects such as acid-base and physical and chemical properties of substances are not very suitable. Then, according to the results of Hadisaputra (2017) research ChemLab software is also able to represent macroscopic aspects to bridge chemical practices in the laboratory, such as colour changes, and phase changes, such as liquids, gases and solids.

From this explanation, it can be seen that computational chemistry can be used as an alternative learning medium to help improve students' understanding of chemical materials optimally (Arifani, et al., 2021). Computational chemistry can support concrete chemistry learning, and learners in hands-on experience in rotating and translating structures. 3D visualization strengthens submicroscopic level illustrations (Pernaa, 2022). The same thing was also explained by Prianto (2007) computational studies to understand the properties and changes in macroscopic systems through simulations based on the laws of interaction that exist in the system. For example, the properties of molecules (energy, structure, dipole moment, polarity, or hyperpolarization) can be included in the calculations.

Previous research by Marwan and Nugraha (2022) stated that learning media with computational methods on haloalkane material got an average percentage of 92.6%, which means that it is very feasible to use. Similarly, research on learning media based on computing methods using *NWChem Software* on electrolyte and non-electrolyte solution materials obtained an average percentage of 87.50% with a very feasible category (Harahap, et al., 2022)

Based on the results of Hasibuan, et al., (2020) that the use of *NWChem software* in learning molecular shape material makes a very high contribution compared to using *Chemsketch software*.

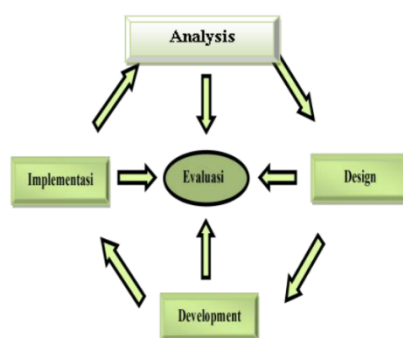
Learning media using *NWChem* can improve student learning outcomes because in this media students can learn molecular shapes with images and video animations of the molecular shapes.

Research conducted by Sinaga (2021) using Avogadro software, explains that this software can bring students closer to molecules, reveal details at the microscopic level, and better understand the laws of chemistry, chemical properties, chemical reactions, and other chemical phenomena. Meanwhile, research by Hasby (2018) concluded that the use of visualization media using *Avogadro software* to describe molecular shapes in 3 Dimensions (3D) has been proven to attract students' interest in learning and understanding. This software can clarify the understanding of abstract concepts so that it can be more concrete, easy for students' brains to capture and fun to follow the explanation.

Following the characteristics of the basic competencies of hydrocarbon materials and the needs of media in the teaching and learning process, the use of computational chemistry with *Avogadro*, *NWChem*, and *Jmol* software is suitable to be applied to achieve learning goals. The purpose of this study is as an initial study of information collection in the context of analyzing the need to design a draft of learning media based on computational chemistry assisted by *Microsoft Sway*. Needs analysis is carried out through literature studies and field studies. Literature study by observing the school curriculum and learning media that have been used so far. Field studies are carried out by providing questionnaires on the needs of learning media and interviews.

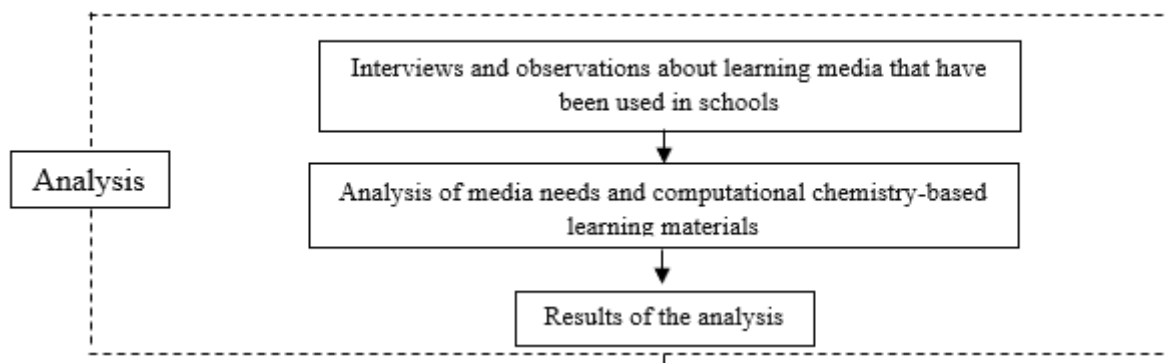
## 2. Research Methodology

This research is a type of research *and development* (R&D). The ADDIE model is the researcher's choice because at the stage of the ADDIE model provides an opportunity to evaluate development activities at each stage. The ADDIE model consists of the *Analysis*, *Design*, *Development*, *Implementation*, and *Evaluation* stages. This can be seen in Figure 1.



**Figure 1.** ADDIE model development flow

The first stage in this study is the analysis stage, this stage is the information collection stage. The methods used in the initial information collection are literature studies and field studies. This can be seen in Figure 2.



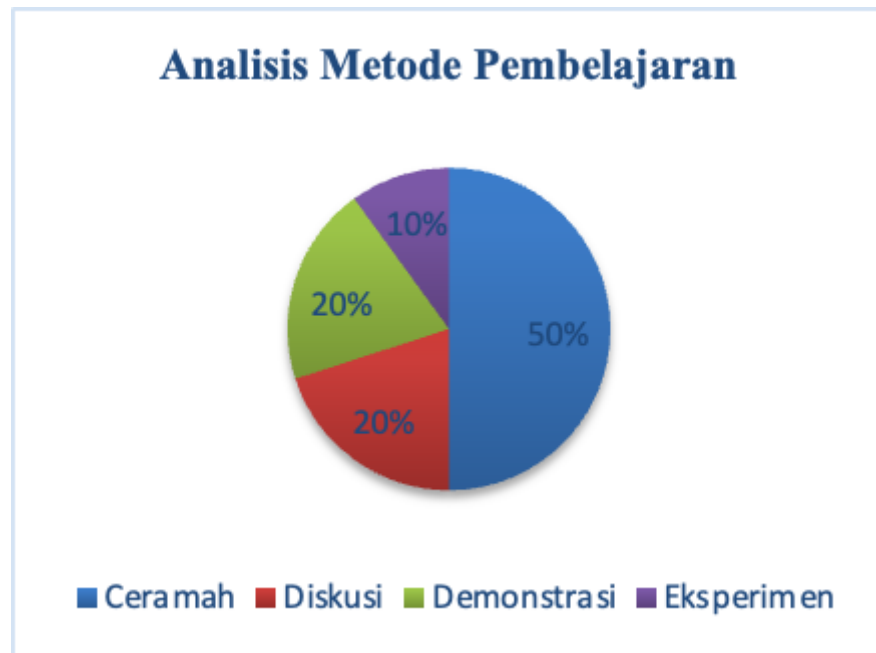
**Figure 2.** Analysis Stage

The literature study is carried out by collecting relevant research and sources and reviewing the curriculum, syllabus, and basic competencies in chemistry which will be the basis for the development of computational chemistry-based learning media while the field study is carried out by providing a questionnaire on media needs and interviews with chemistry teachers at high school SMA Negeri Modal Bangsa Arun, Lhokseumawe City.

### 3. Result and Discussion

Needs analysis as the basis for the development of computational chemistry-based learning media is an initial activity carried out before developing computational chemistry-based learning media. The analysis carried out at the beginning was a literature study, curriculum analysis, syllabus analysis, learning media analysis, and teaching material analysis on hydrocarbon materials. The results of the analysis obtained are used as a reference to develop learning media based on computational methods on hydrocarbon materials. Material analysis is carried out to mark, summarize, and structurally arrange chemical objects such as facts, concepts, and procedures on hydrocarbon materials that students will learn.

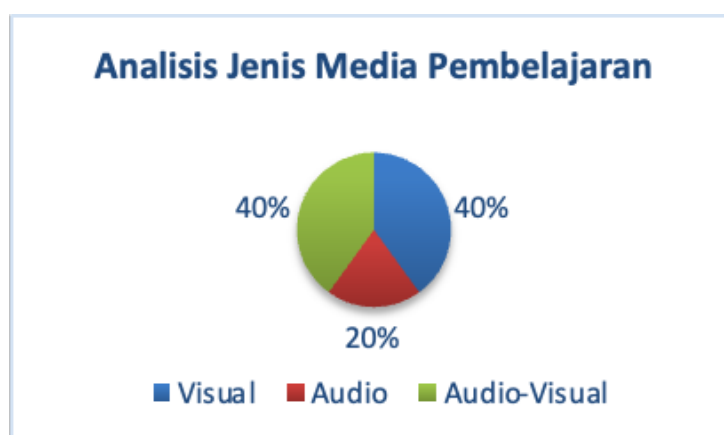
The next analysis is a field study to find out the learning process, the media used during the learning process, the learning methods used, and the need for computational chemistry-based learning media. Questions about learning methods are aimed at finding out the learning methods that teachers most often use during the teaching and learning process. The results can be seen in Figure 3.



**Figure 3.** Analysis of Learning Methods

Based on these results, it was found that the lecture method is the most frequently used in the learning process carried out by 3 teachers as respondents. The lecture method is often also called the conventional method. This method is still widely used by teachers as a way to convey material to students. Although this method is more criticized because teachers are active while students are passive, it cannot be eliminated in the learning process, because it is still needed or this method still has advantages under certain conditions (Lufri, et al., 2020). However, for this method to still be used by teachers, teachers should use tools or media that can support the learning process under the goals to be achieved.

The next question is about the type of learning media that has been used by teachers. It can be seen from Figure 4.



**Figure 4.** Analysis of Types of Learning Media

Based on the analysis of the types of learning media that have been used by teachers, it was found that the use of visual and audiovisual media types has the same percentage of 40%, meaning that the types of images and videos that are often used in the learning process so that students are interested in learning. Visual media is a type of media that relies only on students' sense of sight, so the learning experience received by students is highly dependent on their visual abilities such as books, journals, posters, photos, the surrounding nature and so on. Meanwhile, audiovisual media is a type of media used in learning activities by involves hearing and vision at the same time in one activity process. Messages and information that can be channelled through this media can be in the form of verbal and nonverbal messages that rely on sight and hearing (Sumiharsono, R. & Hasanah, H., 2017).

The next analysis is how the teacher conveys hydrocarbon material that can explain the structure or molecules of a compound microscopically. The results were obtained that teachers are still unable to explain the structure or molecules of a compound microscopically due to the lack of learning media that can meet the learning objectives. So far, teachers have only used the molimod model or presented images taken from internet sources. The books used in the learning process also do not present three-dimensional images of structures or molecular shapes. So this is an obstacle for students to improve their knowledge in depth. Based on research by Lubis and Rahmania (2022), it is explained that the use of computer multimedia in hydrocarbon learning has a greater influence than being taught directly by teachers because with the use of multimedia students can remember and understand several contextual concepts.

Furthermore, based on the questionnaire for the analysis of teachers' needs, they also attached a written statement regarding teachers' obstacles in making learning media, especially based on computational chemistry. Teachers revealed that the time needed to make learning media is very much while teachers do not have much time due to various busyness at school. As well as a lack of knowledge of teachers in making media based on computational chemistry because it is rare to hold training on making media that can support microscopic learning. Therefore, 100% of teachers stated that the use of computational chemistry-based learning media in the learning process needs to be developed.

#### **4. Conclusions**

Based on the results of the needs analysis as the basis for the development of computational chemistry-based learning media, it can be concluded that teachers need computational chemistry-based learning media on hydrocarbon materials so that students understand the concept microscopically. The results of this study are only used as a reference for research with the same topic, namely the development of computational chemistry-based learning media on the subject of hydrocarbons.

## References

- Amalia, Irma., et al., (2019). Pemodelan Reaksi Hidrogenasi Senyawa Hidrokarbon Golongan Alkena dan Alkuna Melalui Studi Komputasi. *CHEMICA: Jurnal Pendidikan Kimia dan Ilmu Kimia*. **2:1** 33-40.
- Arifani, Dewi., Lalu Rudyat, et al., (2021). Pengembangan Modul Praktikum Kimia Berbasis Kimia Komputasi Pada Materi Asam Basa. *Prosiding SAINTEK*. Mataram: 9-10 November 2020. Hal 660-666.
- Hadisaputra, S., Savalas, L. R. T., & Hamdiani, S. (2017). Praktikum Kimia Berbasis Kimia Komputasi Untuk Sekolah Menengah Atas. *Jurnal Pijar MIPA*, 12(1), 11-14.
- Harahap, Annisa Sabbilla., Erlin Karya., & Nugraha Asep Wahyu. (2022). Pengembangan Media Pembelajaran Berbasis Metode Komputasi Pada Materi Larutan Elektrolit dan Non elektrolit. *Educenter: Jurnal Ilmiah Pendidikan*. **1:6** 683-690
- Hasby (2018). Pengaruh Software Visualisasi Terhadap Hasil dan Minat Belajar Siswa Pada Materi Bentuk-Bentuk Molekul di SMA Negeri 4 Langsa. *KATALIS Jurnal Pendidikan Kimia dan Ilmu Kimia*. **1:1** 17-21.
- Hasibuan, Siti Rohaniah., et al., (2020). Development of Learning Media Based on Computation Methods in Molecular Shape. *Proceedings AISTEEL*. 107-112.
- Iskandar. (2002). Pengembangan Lembar Kerja Peserta Didik Berbasis STEM Pada Materi Termokimia. *JS (Jurnal Sekolah)*. **6:332-36**.
- Lubis, Ervi Lutfhi S.W, dan Sri Rahmania., (2022). The Effectiveness of Contextual Teaching and Learning with Multimedia to Increase Student's Achievement on Hydrocarbon Topic. *Lavoisier: Chemistry Education Journal*. 1:1.
- Luciano, E.H., et al., (2014). 3D Printing in the Chemistry Curriculum: Inspiring to Be Creative Innovators. *ACS Symposium Series*, Vol 1180. Chapter 9, 125-146.
- Lufri, et al., (2020). *Metodologi Pembelajaran: Strategi, Pendekatan, Model, Metode Pembelajaran*. Purwokerto: CV. IRDH
- Marwan, Anastasia Gayatri & Nugraha Asep Wahyu. (2022). Pengembangan Media Pembelajaran Menggunakan Metode Komputasi pada Sub Pokok Bahasan Haloalkana di SMA. *Jurnal Ilmiah Multidisiplin Indonesia*. **1:7** 927 -934. E-ISSN: 2809-1612, P-ISSN: 2809-1620.
- Nasution, Annisa, et al., (2023). The Influence of Computation Implementation in Chemistry Basic Courses on Chemistry-Biology Pre-Service Teachers of UIN SyekhAli Hasan Ahmad Addary Padangsidempuan. *Lavoisier: Chemistry Education Journal*. **2:2** 72-77.
- Nurfajriani, Siti, H., & Nur, H. (2020). The Effect of Multimedia *Articulate Storyline* Based on *Discovery Learning* on Creative Thinking Ability in Material Reaction Rate. *Prosiding Seminar Nasional Kimia Berwawasan Lingkungan*. 75-80.
- Paramita, Sari., et al., (2020). Pemilihan Metode Perhitungan Kimia Komputasi Semiempiris untuk Pengembangan 1,3,4-Thiadiazole. *Indonesian Journal of Chemical Research*. **8:1** 51-56.



- Pernaa, Johannes. 2022. Possibilities and Challenges of Using Educational Chem Information for STEM Education: A Swot Analysis of a Molecular Visualization Engineering Project. *Journal of Chemical Education*, 99, 1190-1200.
- Prianto, Bayu. (2007). Pemodelan Kimia Komputasi. *Jurnal LAPAN*. **8:1** 6-9.
- Setyarini, et al., (2022). In-House Training of 3D Molecular Modeling using Avogadro for High School Chemistry Teachers. *Journal of Social Research and Community Service*. **1:1** 15-22.
- Sinaga, Cinthia Uly Hotnami & Nugraha, Asep Wahyu. (2021). Determining the Most Stable Structure of Benzamide Derivatives Using Density Functional Theory (DFT). *Indonesian Journal of Chemical Science and Technology (IJCST-UNIMED)*. **4:2** 49-54.
- Siregar, Anggi Desviana., & Harahap, Lenni Khotimah. (2020). Pengembangan E-Modul Berbasis *Project Based Learning Terintegrasi Media Komputasi Hyperchem* Pada Materi Bentuk Molekul. *Jurnal Penelitian Pendidikan Sains*. **10:1** 1925-1931.
- Sumiharsono, Rudy & Hasanah, Hisbiyatul. (2017). *Media Pembelajaran*. Jember: CV. Pustaka Abadi
- Wiratmojo, P & Sasonohardjo. (2002). *Media Pembelajaran Bahan Ajar Diklat Kewidyaiswaraan Berjenjang Tingkat Pertama*. Lembaga Administrasi Negara.
- Zuliatin, Qonik., Fatayah., & Yuliana, Ika Farida. (2022). Pengembangan E-LKPD Berbasis STEM Pada Materi Struktur Atom. *Journal of Chemical Education*. **11:3** 195-202.