

## Using 3D molecular structure simulation to develop chemistry competence for Vietnamese students

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### Abstract

The spatial structure of organic compounds (3D molecular structure) acts as an important tool in teaching organic chemistry. This study designed 16 3D molecular structures of hydrocarbons and chemical reaction simulations, using these simulations to design teaching plans for alkenes; guide teachers on how to use the teaching plans; and develop tests to assess students' chemistry competency. The research aimed to evaluate the impact of using 3D molecular structure simulations on students' development of chemistry competency. The methodology was conducted on 630 Vietnamese students divided into two groups: an experimental group and a control group. The results of this study have demonstrated the benefits of 3D molecular structure simulation, including enhancement of students' chemistry competency, promotion of transfer and application of spatial chemistry content to higher-order concepts, and expansion of the planning of the nature and mechanism of chemical reactions. As a result, chemistry teachers can use 3D molecular structure simulation to teach topics such as atomic radius, bond length, and bond angle. This research makes an important contribution to the application of technology in teaching and developing chemistry competence for Vietnamese high school students.

**Keywords:** simulation, 3D molecular structure, chemistry competency, Vietnamese students

## INTRODUCTION

### Chemistry Competency

Vietnam's education system is entering a period of fundamental and comprehensive reform, shifting away from a focus on knowledge towards a comprehensive development of learners' quality and competency. Competency is defined in the new general education curriculum 2018, Vietnam as "the ability to apply knowledge, experience, skills, attitudes, and interests to act appropriately and effectively in diverse situations of life"; "chemical awareness; learning about the natural world from a chemical perspective; applying acquired knowledge and skills" have been identified as necessary competencies for students in the new general chemistry curriculum (Ministry of Education and Training, 2018). To evaluate the influence of using 3D molecular structure simulation on the development of students'

chemical competence based on the new general chemistry of Vietnam, the article identifies the expression of three component competencies of chemical competency to build chemical competency evaluation criteria (Table 1).

In Vietnam, along with the innovation of the general education curriculum, many studies that support teaching to develop students' competency have been carried out, such as applying the process of hands-on method (La main à la pâte [LAMAP]) to design the plan and organize Ethyl alcohol lesson, initially evaluated the feasibility of the method and contributed to the development of natural inquiry competency for secondary school students (Thin, 2019); presenting measures to develop students' competency to understand the natural world through the use of WebQuest in project teaching to study the presence of chlorine in domestic water (Thi et al., 2019); design self-

**Contribution to the literature**

- The study evaluates the role of the 3D molecular structure of organic compounds in developing chemistry competence for Vietnamese students.
- The study contributes to an understanding of how structural properties affect the understanding chemical cognition.
- The study provides a way to apply structural knowledge to explain the properties of substances and apply knowledge in real-life scenarios.

**Table 1.** Expression of three component competencies of chemical competency on new general chemistry of Vietnam

Component	Expression
Chemical awareness	Be aware of basic knowledge of substance structure, chemical processes, forms of energy, & energy conservation, as well as some basic chemical reactions & transformations.
Learn about natural world from a chemical perspective	Observe, collect data, analyze, explain, & predict results of natural phenomena & daily life situations.
Apply acquired knowledge & skills	Apply acquired knowledge & skills to solve problems in studying, researching, & real-world situations.

study activities on chemistry subject to develop the competencies for high school students (Cam, 2018); Research on the general structural framework of teaching competency and integrated teaching competency by natural science teachers in general education (Thi, 2021).

In the world, many scientists are interested in developing students' competency. Lu et al. (2013) suggested using mind maps and mind manage software to improve students' competency in solving chemistry problems during the transition period of chemistry instruction in China. Everwijn et al. (1993) instructed students to learn how to apply heuristics in the area of general skills and synthesis skills by interacting with other specialized learning content. In addition, there have been several studies that have addressed the issue of teaching and developing competency to apply learned knowledge and skills, such as Victoria and Paul's (2014) research on the effects of integrated teaching methods on the learning outcomes of chemistry students. León et al. (2018) published research on the relationship between learning management and teacher interaction that can impact the quality of teaching and students' self-study competency. The application of 3D technology in teaching has been widely used to facilitate students' comprehension of the virtual world of matter. In particular, simulations can aid in predicting protein structures from amino acid chains, as well as investigating nanomaterials. Simulation and editing tools have been employed to construct or modify 3D molecular structures (Mazumdar & Shah, n. d.). Simple distance geometry and MMFF force field-based structure optimization have been utilized to generate 3D models (Yamada et al., 2006). Molecular simulations have been employed to elucidate the principles of molecular recognition that cannot be observed through experimental methods (Michel, 2014). Furthermore, deep learning models have been developed to construct 3D molecules capable of binding to target proteins.

These models are trained on atomic density grids of protein-ligand structures and employ appropriate atomic and bonding procedures to produce valid molecular structures from the generated atomic density grids. The potential applications of such models in the field of drug discovery are immense and include the creation of new molecules with the ability to bind to target proteins, thereby reducing the time and cost associated with drug development (Ragoza et al., 2022). However, to the best of our knowledge, there is no research on the method of using 3D molecular structure simulation of organic compounds in teaching chemistry to develop competence for Vietnamese high school students.

**Molecular Structure Simulation**

To achieve the goal of teaching and developing students' competency, it is necessary to innovate concerning objectives, content, and teaching methods. One such method is the use of 3D molecular structure simulations as a visual teaching method, which has been evaluated and found to have many benefits. Many studies have been published on the use of simulation in teaching chemistry, such as building simulations of molecular structures. Some virtual models have been made publicly available by PhET, Colorado University (Moore et al., 2014). Studies on multimedia learning in online learning environments show that the effectiveness of 3D molecular structure simulations in supporting student learning depends on several factors (Höffler & Leutner, 2007). Research has shown that spatial ability plays a role in students' learning in the context of multimedia learning (Heo & Toomey, 2020; Sanchez & Wiley, 2006). The spatial ability allows us to manipulate and understand spatial relationships in both real and virtual spaces and is often used when completing everyday tasks such as assembling furniture or navigating to different locations. However, much of

the research on spatial ability has been conducted using multimedia in which participants do not interact with the multimedia (Sanchez & Wiley, 2014), and there is a need for further research on the role of students' spatial ability in learning from interactive multimedia, such as virtual modeling (Stull & Hegarty, 2016).

In the field of chemical science, chemical reaction structures and processes occur on a microscopic scale that is invisible to the learner. Therefore, 3D molecular structure simulation of chemical compounds plays an important role in teaching. Chemistry teachers can use physical models or simulations to help students visualize and understand concepts in a virtual environment (Stieff, 2011; Stieff & Wilensky, 2003). Simulations allow the user to observe patterns of chemical molecules and reaction processes that are normally invisible to the naked eye (Plass et al., 2009). They support students' study of the scientific content of organic compounds.

According to Johnstone (1991), chemistry learning occurs at three levels: macroscopic, which can be experienced with our senses; submicroscopic, which includes atoms, molecules, and ions; and symbolic representation, which includes structural and empirical formulas and chemical equations. To deeply understand the nature of chemistry, it is necessary to assist learners in studying micro-level chemical content. Many studies have focused on identifying supporting theoretical frameworks for complex 3D molecular structures (Stieff et al., 2016). The results of these studies show that 3D molecular structure simulations help learners consolidate their understanding and increase reasoning. Learners who have only been observed without interacting with molecular simulations have a firmer understanding than those who have not been observed (Padalkar & Hegarty, 2015; Stull & Hegarty, 2016).

How can multimedia files such as simulations be effective in teaching? This issue has been addressed by many studies, which examine the fair use of images and text according to the principle of multimedia (Fletcher & Tobias, 2005; Mautone & Mayer, 2001). Learners have a better cognitive experience when text is adapted into audio, images, and videos (Brünken et al., 2004; Mousavi et al., 1995). Visual images, such as maps, are more effective when used before scientific text (Kulhavy et al., 1993). Technology tools are a very effective means of supporting online teaching, especially interactive technology (Daher et al., 2022).

On the construction and use of molecular simulations of chemical compounds, Casselman et al.'s (2021) research compared the effectiveness of teaching stereochemistry using physical models and using virtual models. The study also suggests that scientific content should use virtual models and the role of students' spatial skills in learning.

Some general principles when designing images and simulations used in teaching have been developed based on research on multimedia teaching (Mautone & Mayer, 2001; Moreno, 2006). Intuitiveness and the ability to transmit diverse, flexible information are the fundamental principles of simulation design in teaching. Some of the theoretical principles and experiences presented by Weiss et al. (2002). Visual design principle: the animation must be realistic, vivid, and transformed over time (Hegarty, 2004).

The principle of interaction design is to allow learners to control the tempo and sequence of the evolution of the simulation. Interactivity is divided into three levels: control of the provision of information (such as pause buttons, and fast forward ...), interaction with content (setting the parameters of the simulation), and content interaction (e.g., rotation, change the position of objects) (Garg et al., 2001; Kalyuga, 2007; Kennedy, 2004). The students used mental rotation most frequently in identifying 2D chemical structural formulas and used mental rotation less frequently to rotate 2D figures. The students used similar mental rotation strategies in identifying 3D objects and chemical structural formulas, but the high-achieving students performed better in identifying 3D objects and 3D chemical structural formulas because of the multiple and useful strategies of mental rotation (Huang & Liu, 2012).

The use of a locally produced hypermedia instructional package has been shown to significantly improve the post-test performance of chemistry students. Additionally, the use of these instructional packages also resulted in a significant improvement in students' retention ability test scores, as shown in a study by Oluwafemi (2016).

In this study, we aim to evaluate the impact of 3D molecular structure simulations of organic compounds on teaching and developing chemical competency in students. We will investigate the effects of understanding structural properties on chemical cognition and the ability to apply structural knowledge to explain the properties of substances and apply knowledge in real life. Our research will focus on answering the following questions:

1. How do Vietnamese teachers currently utilize 3D molecular structure simulations in their teaching of chemistry?
2. How can 3D molecular structure simulations be used to develop students' chemistry competencies effectively?
3. How is the student's chemical competency improved after teachers use the simulations to analyze 3D structure in teaching the hydrocarbon section?

**Table 2.** Design principles

Step	Objective	Results
1	Research published findings related to 3D molecular structure simulation and its impact on student competency development in teaching chemistry.	This study examines the effects of using 3D molecular structure simulations on students' competency development in chemistry education.
2	Develop a survey to assess the current usage of 3D molecular structure simulation in teaching chemistry.	A total of 283 chemistry teachers participated in the survey to gather information on current practices and perceptions of using 3D simulations in teaching.
3	Develop 3D molecular structure simulations as teaching tools, design teaching plans, assist teachers in experimenting with these plans to enhance student chemistry competency, and create rubrics to evaluate competency through review sheets and tests.	Sixteen 3D simulations, two teaching plans (consisting of four periods each), and three chemistry competency assessment tests were developed and used in the study.
4	Conduct experiments at 14 Vietnamese high schools in various regions, urban/rural and mountainous. The students participated in the experiments in the North, Central and South of Vietnam, with 630 grade 11 students divided into two groups: a control group (N1) and an experimental group (N2). Administer three tests to assess chemistry competence for all 630 students.	The teachers in the experimental group (N2) taught four lessons on alkanes and alkenes using the provided teaching plan and simulations, while the control group (N1) received traditional instruction, the same was true for the four lessons of N2.
5	Analyze the test results and evaluate the impact of using 3D molecular structure simulations in teaching on the development of chemistry competence among students.	Results were gathered through the administration of three competency assessment tests before and after the intervention. The results showed that, before the intervention, both the N1 and N2 groups had equivalent chemical competency. However, after the intervention, the N2 group exhibited a higher level of chemical competency compared to the N1 group.

## METHOD

### Overview of Study Design

This research follows the principles listed in **Table 2**.

#### *Develop a survey*

We developed a teacher survey to determine the current usage of 3D molecular structure simulation in teaching chemistry. The survey included three main areas of inquiry:

- (1) the sources of 3D molecular structure simulation used by teachers in teaching chemistry,
- (2) teachers' self-assessment of their degree of use of 3D molecular structure in teaching, and
- (3) the challenges teachers face when using simulations in teaching chemistry.

283 chemistry teachers participated in the online survey, which was conducted using Google Forms (**Appendix A**). The survey results were statistically analyzed using SPSS 22.0 software. These results provided the research team with a basis for proposing the development of teaching plans using 3D molecular structure simulations for the experimental group (N2). The results of the survey are presented.

#### *Develop 3D molecular structure simulations*

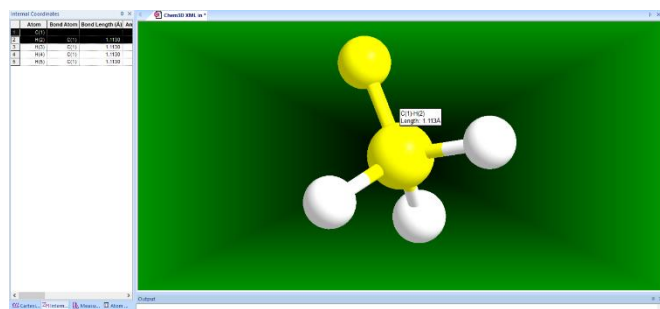
In a published study, Plass et al. (2009) emphasize the principle of visualization and interaction when

designing simulations. Based on the study of the role of 3D molecular structure in developing students' chemical competence and the current status of using simulations in teaching, we propose principles for designing simulations of the molecular structure of organic compounds, including

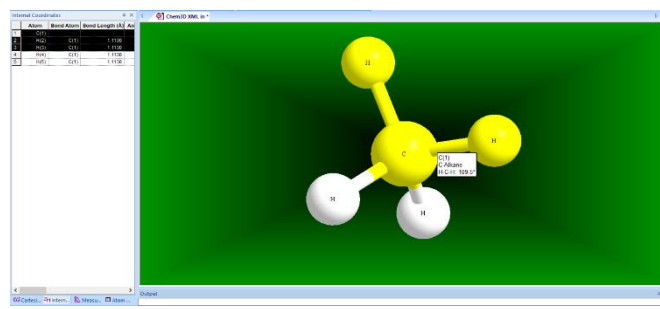
- (1) depicting the structure of molecules that cannot be seen by the naked eye,
- (2) the simulation reflecting some of the structural information such as bond length, bond angle,
- (3) simulating chemical reactions and specifying the mechanism of the reaction,
- (4) designing simulations to be uniform in color and image, depicting the true nature of science, and
- (5) incorporating minimal interactivity, allowing students to pause, review, and zoom in.

To conduct the construction of simulations of organic compound molecular structure, we use the ChemBio 3D Ultra 12.0 tool in the ChemBio Office 2010 software (Cambridgesoft, 2021). The software enables us to set up a simulation of the 3D structure of organic compound molecules and determine some molecular structure information such as atomic radius, bond length, and bond angle.

Methane (**Figure 1**) is the first molecule in a series of alkanes, consisting of compounds containing only carbon and hydrogen in which the molecule contains only single bonds (Crabtree, 1995). The H-C-H bond angle is 109.5 degrees (**Figure 2**).



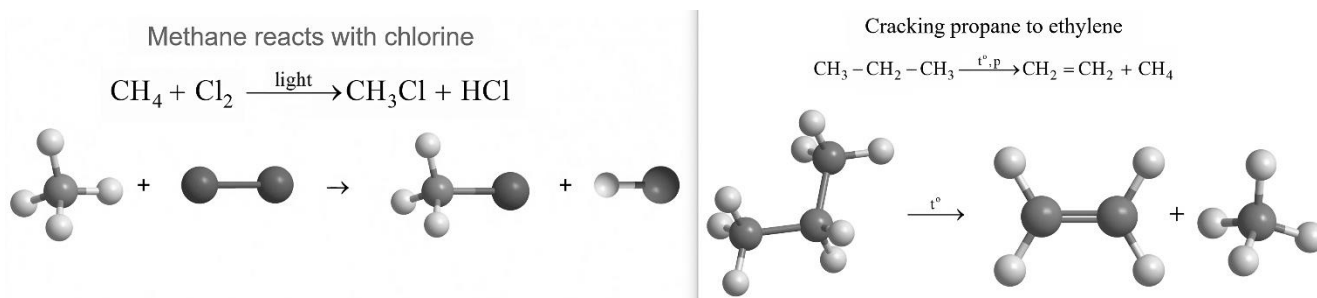
**Figure 1.** C-H bond length (Source: Authors' own elaboration)



**Figure 2.** H-C-H Bond angle (Source: Authors' own elaboration)

**Table 3.** Comparison between methane & ethane

Link length & angle	CH <sub>4</sub>	C <sub>2</sub> H <sub>6</sub>
C-H bond length	1.113 Å	1.113 Å
H-H distance	1.8118 Å	1.812 Å (C <sub>1</sub> ) 2.512 Å -3.097 Å (C <sub>1</sub> -C <sub>2</sub> )
H-C-H bond angle	109.5°	109°
C-C bond length		1,523 Å
C-C-H bond angle		110°



**Figure 3.** 3D mechanism of organic reactions (Source: Authors' own elaboration)

Ethanes are the second substance in the series of alkanes, which are compounds containing only carbon and hydrogen. They have structural parameters similar to methane. By taking the same steps, we identified the structural parameters of both methane and ethane (Table 3).

For simulating the mechanisms of organic reactions, we utilized the ChemBio 3D Ultra 12.0 tool in the ChemBio Office 2010 software (Cambridgesoft, 2021) to design atomic images and Microsoft PowerPoint 2019 to create animations (Figure 3). In the process of designing animations, we visually described the cleavage and bond formation, reflecting the theoretical basis of organic reaction mechanisms. We developed simulations of the substitution reaction mechanism of chlorine in alkanes, bromine, and propane; the mechanism of addition reactions of hydrogen and bromine to alkenes; and the mechanisms of separation, cracking, and polymerization reactions.

Similarly, we designed 10 simulations of the molecular structures of some alkenes and the mechanisms of organic reactions. These simulations are all published in video format and uploaded to YouTube for the convenience of teachers and students to observe.

After designing the simulations, we trained teachers and students on how to use the 3D molecular structure simulations in their teaching and learning process to develop students' chemical competencies (Appendix B).

#### Develop a plan for each topic

Teaching plans have been designed to meet the requirements of the Vietnamese general education curriculum and ensure flexibility in implementation to suit the specific conditions of each locality and general education institution. The plans promote initiative and creativity in the implementation of the lesson, and effective use of teaching facilities and equipment to meet the requirements of implementing teaching methods, testing, and evaluation according to the requirements of developing students' qualities and competencies.

In Vietnam's curriculum of chemistry program, students learn about the molecular structure of organic compounds, followed by learning about alkanes and alkenes as properties are closely related to molecular structure. Therefore, the research focuses on alkane and alkene topics (as outlined in Appendix C). Each topic has a duration of two lessons (90 minutes) and the objectives of the teaching plans must meet the requirements of nine criteria on chemical competence. Tasks of teachers and

**Table 4.** Scale of thinking levels

Thinking levels	Describe
Recall/recognition	Students can recall and recognize basic concepts when asked.
Comprehension/understanding	Students can understand and comprehend basic concepts and apply them to examples presented in a similar manner as taught by the teacher or in the classroom.
Application lower level	Students can comprehend concepts at a higher level and make logical connections between basic concepts and can manipulate them to organize information that is presented similarly to the teacher's lecture or in the textbook.
Application upper level	Students can use their subject or topic knowledge to solve new, non-similar problems, that are appropriate and require the use of acquired skills and knowledge. These are problems that are similar to situations students may encounter in society.

**Table 5.** Standard output of students' competencies

CC	A	Content
Chemical awareness	C1	Recognize and name chemical objects, events, and concepts.
	C2	Present facts, characteristics, and roles of objects and chemical concepts.
	C3	Analyze aspects of chemical objects, concepts, or processes according to a certain logic.
	C4	Compare, classify, & select objects, concepts, or chemical processes according to different criteria.
	C5	Explain and reason about relationships between objects, concepts, or chemical processes (structure-properties & cause-effect).
Learn about natural world from a chemical perspective	C6	Propose problems: Recognizing and asking questions related to the problem; analyzing the context in which the problem is proposed; expressing problems.
	C7	Implement a plan: gather facts and evidence (observations, notes, data collection, experiments); analyze data to prove or disprove a hypothesis; draw conclusions and adjust as necessary.
Apply knowledge & skills learned	C8	Apply knowledge of chemistry to explain various natural phenomena and applications of chemistry in everyday life.
	C9	Demonstrate appropriate behavior in situations related to self, family, and community, in line with the requirements of sustainable social development and environmental protection.

Note. CC: Component competency & A: Abbreviation

students are specifically assigned, and activities are designed explicitly.

The teacher implements the lesson plan and the student's task is to preview the simulation, perform tasks in the study sheets, conduct tests, etc. Teaching activities include experiencing activities, connecting; new knowledge-forming activities (learning about molecular structure characteristics, learning homologs, isomers, and nomenclature, understanding and predicting and explaining physical properties, forming knowledge about chemical properties, learning applications, and modulation); practicing activities – test and assess competencies.

Teachers use the reverse classroom method to teach the topics that have been built-in, either in person or online. Students are tasked with previewing the simulations and completing worksheets before class. During class, students exchange and discuss the researched content and synthesize their knowledge.

#### *Building rubrics and tests that assess students' chemistry competencies*

Using a scale of levels of thinking developed by Boleslaw Niemierko (Gajek, 2019), we propose and describe in detail each criterion at four levels of expression. These levels can be listed in the following ways:

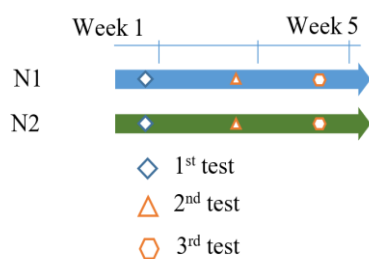
1. Level 1: Recall/recognition,
2. Level 2: Comprehension/understanding,
3. Level 3: Application lower level, and
4. Level 4: Application upper level (**Table 4**).

Using this scale to develop rubrics that assess a student's chemistry competency.

Rubrics and the student chemistry competency test are used as assessment tools that are built according to four levels of expression corresponding to each criterion. To construct a rubric to evaluate chemistry competence for the alkane and alkene topics, we establish students' competency output standards with specific criteria (C1 to C9) (**Table 5**).

The test to assess students' chemical competency is designed based on the outcome standards that students need to achieve in the lesson objectives. The tests have similar scales and assessment tools; each exam consists of 10 questions allocated to assess the competency of the component: chemical cognitive competency (questions 1 to 4); competency to understand the natural world from a chemical perspective (questions 5 to 8); competency to apply knowledge and skills learned (questions 9 and 10).

The questions are presented in the form of objective multiple choice with four options, each option corresponds to a level according to the rating scale of



**Figure 4.** Progress of time (Source: Authors' own elaboration)

thinking levels. All students take the test on Google Forms in 15 minutes.

## Experimental Teaching

### Experimental process

First, we developed survey questions and sent the questionnaire to experts for comments. Then, we prepared a lesson plan, reviewed it, and had teachers conduct trial lessons. We adjusted the teaching plan and sent it back to the experimental teachers to conduct the experiments. The experimental lessons were recorded. Finally, students were assessed using rubrics and competency tests. The research results were analyzed, evaluated, and compared to the outcome standards of students' competency.

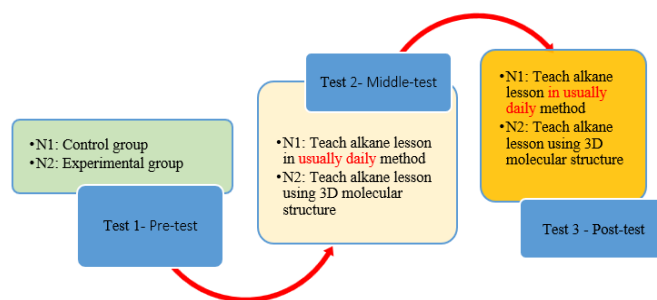
The school year in Vietnamese high schools lasts nine months, from September of the previous year to May of the following year. The experiment was carried out at high schools for five weeks, following the professional plan prescribed by Vietnam Ministry of Education the content of the research's lessons, and the progress of the study. Experiments at high schools are depicted in **Figure 4**.

Teachers who were teaching in class with students participating in experiments were guided through the implementation process and provided with enough tools such as lesson plans, tests, and learning materials. The experiment was carried out in the following 3 steps:

**Step 1. Preparation:** Teachers plan to teach in classes, study the provided teaching plan, and prepare necessary equipment such as computers, projectors, and classrooms. Students are grouped, studied, and trained in the steps to implement the experiment.

**Step 2. Experimental teaching:** Lessons are conducted in a flipped classroom format. Teachers provide simulations for students to preview at home. Students view 3D simulations of molecular structures and answer questions on their worksheets. In the classroom, teachers organize learning activities to synthesize the knowledge students have learned on their own and consolidate, apply, and improve knowledge. These steps are carried out following the teaching plan.

The study selects 11<sup>th</sup> grade students who will only learn about hydrocarbon in the experiment. These



**Figure 5.** Experimental teaching process in the classroom (Source: Authors' own elaboration)

students were assessed by chemistry teachers at 14 high schools participating in the experiment to have similar learning results in chemistry. To confirm the teacher's assessment of the learning outcomes of students participating in the experiment, the research was conducted for all selected students to participate in the pre-test (test 1). The number of students participating in the pre-impact assessment is more than 630. However, the study-selected students to participate in the experiment must ensure the following conditions:

1. The results of selected students in test 1 are similar.
2. Students must fully participate in four hours of experimental teaching (as confirmed by the teacher directly teaching the experiment).
3. The students fully participated in all three tests (tests 1, 2, and 3).

The tests are used for both groups N1 and N2. The content of each test includes 10 multiple-choice questions with four options with quantitative levels (recall/recognition=1; comprehension/understanding =2; application lower level=3; and application upper level=4).

Before the experiment, test 1 was used to assess students. To do a progress assessment, we use test 2 in week three, and test 3 in week five (**Figure 5**).

**Step 3. Collecting results and processing data:** The tests are conducted in an online format. Collected results are processed by SPSS 22.0 software, and detailed results are presented.

## RESULTS

### Results of Chemical Teachers' Survey

The survey content includes questions about using teaching materials to support teaching about 3D molecular structure: Using images from textbooks, drawing on the blackboard or using images from the internet, assembling molecular physics models, creating models from simple materials and using virtual molecular models from the Internet or computer software. The survey results from **Table 6**, with the highest score of four points, show that many teachers are

**Table 6.** Sources to create 3D structural simulations used in teaching chemistry

No	Questions	n	Mean	Standard deviation
Q1	Pictures in textbook	277	3.112	0.7744
Q2	Draw into blackboard or use pictures	277	2.957	0.7928
Q3	Pictures from the Internet	277	2.166	0.9750
Q4	The assembled molecular model	276	2.011	0.9244
Q5	Make models from simple materials	280	2.939	0.7896
Q6	Virtual models via the Internet, web, etc.	283	2.211	1.0152
Q7	Molecular model created from computer software	279	1.953	1.0464

Note. Level: Never=1; Occasionally=2; Frequently=3; & Always=4

**Table 7.** Results of teachers' evaluation of the level of media use in chemistry teaching

No	Questions	Level 1		Level 2		Level 3		Level 4	
		A	%	A	%	A	%	A	%
Q1	Pictures in textbook	2	0.7	66	23.8	111	40.1	98	35.4
Q2	Draw into blackboard or use pictures	6	2.2	75	27.1	121	43.7	75	27.1
Q3	Pictures from the Internet	80	28.9	103	37.2	62	22.9	32	11.5
Q4	The assembled molecular model	94	34.1	107	38.8	53	19.2	22	8.0
Q5	Make models from simple materials	6	2.1	78	27.9	123	43.9	73	26.1
Q6	Virtual models via the Internet, web, etc.	82	29.0	94	33.2	65	23.0	42	14.8
Q7	Molecular model created from computer software	124	44.4	79	28.3	41	14.7	35	12.5

Note. A: Amount; Level: Never=1; Occasionally=2; Frequently=3; & Always=4

**Table 8.** Difficulty factors when using 3D molecular structure simulation in teaching organic chemistry

No	Questions	n	Mean	Standard deviation
Q8	Lack of computer	283	0.459	0.4992
Q9	Lack of software, lack of simulation	283	0.527	0.5002
Q10	Difficult to access the Internet	283	0.364	0.4820
Q11	Lack of facilities and teaching aids	283	0.562	0.4970
Q12	Teaching aids are not usable	283	0.300	0.4592
Q13	There is no time to prepare lessons	283	0.389	0.4883
Q14	Lack of knowledge & skills in using simulation software	283	0.615	0.4875
Q15	Role of simulation in teaching organic chemistry is not yet understood	283	0.325	0.4692

Note. Level: Never=1; Occasionally=2; Frequently=3; & Always=4

still inactive in preparing teaching materials: Textbooks (average score Q1=3.92), drawing on the blackboard and using pictures (average score Q2=2.957). Teachers rarely used assembled molecular models on average (average score Q4=2.011) or modelled from simple materials (average score Q5=2.939). In addition, using virtual molecular models via the internet or computer software is infrequent (mean score Q6=2.211; mean score Q7=1.953). In **Table 6**, questions from Q1-Q7 are optional, so the number of teachers answering is from 276 to 283 people.

### Results of teachers' evaluation of level of media use in chemistry teaching

To get the results of assessing teachers' use of media in teaching chemistry, the study focused on building four levels (never=1; occasionally=2; frequently=3; always=4) for teachers to choose from 7 questions in the survey. The results obtained in **Table 7** show that 124 teachers (44.4%) chose never to use 3D molecular structure modeling software (Q7, mean [M]=1.953<2.0, below the regular level, **Table 6**). Most of the teachers'

responses were biased towards occasional or never use. Additionally, up to 28.9% and 34.1% of teachers said that they have never used images from the internet or assembled models (Q3, M=2.166; standard deviation [SD]=0.9750 and Q4, M=2.011, SD=0.9244, **Table 6**). From  $SD \leq 1$ , it can be seen that the choices and assertions of teachers are relatively consistent.

In order to determine the reasons why teachers are less likely to use simulations in teaching chemistry, we designed a teacher survey question. The results collected are summarized in **Table 8**.

With selection of factors affecting use of simulation in teaching chemistry, the survey results from 283 teachers showed that the factor of lack of knowledge and skills in using simulation software (Q14, M=0.615) is the most influential factor in the use of simulation in teaching chemistry. Additionally, two other factors, lack of software (Q9) and lack of means and teaching aids (Q11) have the same mean value greater than 0.5 (**Table 8**), which means that these factors are considered by most people to be the most important and difficult factors affecting the process of using simulation in the teaching of chemistry. Also, a large number of teachers have not



**Table 9.** Statistics of students participating in the survey

Gender/district	Student			
	Group 1 (N1)		Group 2 (N2)	
	Count	Row N (%)	Count	Row N (%)
Gender Male	145	46.2	169	53.8
Female	133	42.1	183	57.9
District Urban areas	216	45.9	255	54.1
Rural & mountainous areas	62	39.0	97	61.0

**Table 10.** Correlation between gender, location, & 1<sup>st</sup> test results

Gender/district		Sex	District	Test 1
Gender	Pearson correlation	1	0.031	-0.006
	Sig. (2-tailed)		0.437	0.877
	n	630	630	630
District	Pearson correlation	0.031	1	-0.059
	Sig. (2-tailed)	0.437		0.141
	n	630	630	630
Test 1	Pearson correlation	-0.006	-0.059	1
	Sig. (2-tailed)	0.877	0.141	
	n	630	630	630

**Table 11.** Test results

Test 1	Test 2		Test 3					
	Mean (N1)	Mean (N2)	Mean (N1)	Mean (N2)				
T11	2.2	2.6	T21	2.8	3.1	T31	3.1	3.5
T12	3.0	3.2	T22	2.8	3.2	T32	3.4	3.7
T13	3.3	3.0	T23	3.2	3.4	T33	3.2	3.5
T14	3.1	2.7	T24	3.2	3.1	T34	3.3	3.8
T15	3.5	3.7	T25	3.3	3.5	T35	3.4	3.7
T16	3.0	3.0	T26	3.0	3.3	T36	3.3	3.7
T17	3.1	3.1	T27	3.3	3.4	T37	3.3	3.5
T18	3.0	3.1	T28	2.9	3.2	T38	3.3	3.6
T19	3.0	3.0	T29	3.2	3.5	T39	3.1	3.6
T110	3.0	2.8	T210	2.7	2.9	T310	3.3	3.7
	<b>3.01</b>	<b>3.00</b>		<b>3.04</b>	<b>3.25</b>		<b>3.28</b>	<b>3.65</b>

yet confirmed the role of 3D molecular structure simulation in teaching (Q15, M=0.325, SD=0.4692), which leads to teachers not frequently using 3D molecular structure simulation in teaching.

**Results of Assessing Impact of Using 3D Molecular Structure Simulation on Development of Chemical Competence of Vietnamese Students**

From the above requirements, the total number of students participating in the experiment was 630, including 314 boys and 316 girls, 471 students from urban areas, and 159 students from rural and mountainous regions (Table 9).

The results of the statistical correlation between the variables of gender and place of residence with the mean value of test number 1 (including two groups of students) are shown in Table 10. Result of Sig. value between gender and first test result is 0.877, and between the place of residence and the first test result is 0.141.

To have a fundamental for assessing students' chemical competencies, besides designing criteria (C1 to

C9) (Table 5), research also design questions to assess students' chemical competencies. The fundamentals for designing the questions in the test include affirming the role of 3D molecular structure simulation, helping students understand the molecular structure and properties of chemical substances and explain the properties of substances, thereby applying knowledge of substances in practical learning.

Criteria table of chemical competencies that need to be formed and developed for students in teaching chemistry (Table 5). For each criterion (C1-C9), there are corresponding chemistry questions. The scores obtained for each criterion in four levels correspond to the scores of 10 questions in three tests, numbers 1, 2, and 3. Chemical cognitive capacity corresponds to five criteria C1- C5; the ability to understand the natural world from a chemical perspective corresponds to two criteria C6 and C7 and the ability to apply knowledge and skills corresponds to criteria C7 and C9. In each test built with ten questions, students' answers are assessed on four levels, respectively, from one to four points. The results are shown in the Appendix C.

**Table 12.** Correlation between study subjects & test results

		Students (n)	Test 1	Test 2	Test 3
Test	Pearson correlation	1	-0.007	0.257**	0.525**
	Sig. (2-tailed)		0.851	.000	.000
	n	630	630	630	630
Test 1	Pearson correlation	-0.007	1	0.028	-0.042
	Sig. (2-tailed)	0.851		0.482	0.291
	n	630	630	630	630
Test 2	Pearson correlation	0.257**	0.028	1	0.155**
	Sig. (2-tailed)	0.000	0.482		.000
	n	630	630	630	630
Test 3	Pearson correlation	0.525**	-0.042	0.155**	1
	Sig. (2-tailed)	.000	0.291	.000	
	n	630	630	630	630

Note. \*\*Correlation is significant at the 0.01 level (2-tailed)

**Table 13.** Paired samples statistics

		Mean	n	Standard deviation	Standard error mean
Pair 1	Test 2TN	3.2517	352	0.40950	0.02183
	Test 1TN	3.0045	352	0.35571	0.01896
Pair 2	Test 3TN	3.6483	352	0.30643	0.01633
	Test 1TN	3.0045	352	0.35571	0.01896
Pair 3	Test 3TN	3.6483	352	0.30643	0.01633
	Test 2TN	3.2517	352	0.40950	0.02183

**Table 14.** Paired samples test

		Paired differences					T	df	Sig. (2-tailed)
		M	SD	SEM	95% CI of difference				
					Lower	Upper			
Pair 1	Test 2TN-test 1TN	0.24716	0.52275	0.02786	0.19236	0.30196	8.871	351	.00003
Pair 2	Test 3TN-test 1TN	0.64375	0.46876	0.02498	0.59461	0.69289	25.766	351	.00018
Pair 3	Test 3TN-test 2TN	0.39659	0.51594	0.02750	0.34251	0.45068	14.422	351	.00043

Note. M: Mean; SD: Standard deviation; SEM: Standard error mean; & CI: Confidence interval

Tests were performed on both experimental and control subjects. The questions were coded as test 1 (from T11 to T110), test 2 (from T21 to T210), and test 3 (from T31 to T310). The results of the tests are summarized in **Table 11**.

The mean score of the two groups is 3.01 (N1) and 3.00 (N2) without much difference, which proves that the subject does not correlate with the results of the assessment of chemical competence of students in test 1.

The correlation between test results and research subjects was determined. The statistical results of the correlation between the variables of the mean value of the test and the research subjects showed that Sig. value between the two groups of students with the first result was  $0.851 > 0.05$  (**Table 12**). The chemical ability of the two groups of subjects prior to the intervention showed no significant difference.

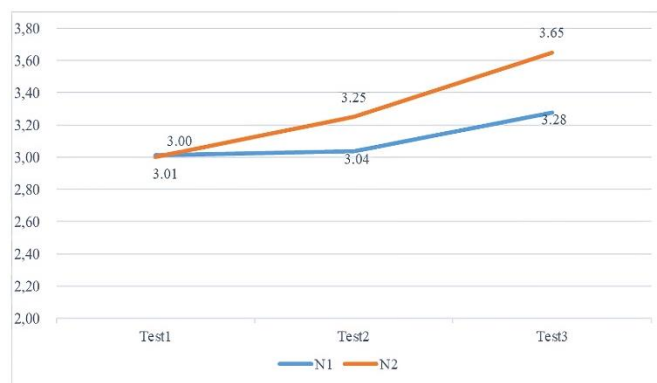
To evaluate the effect of using 3D structural simulation on 352 students in the N2 group, we calculated the mean of three tests, designated as test 1TN, test 2TN, and test 3TN. The comparison table between the mean values of the tests is summarized in **Table 13**.

The results in **Table 14** show that the values of Sig. (2-tailed) are all  $< 0.05$ , indicating that there is a significant difference in the mean of the tests. This proves that the experimental process has an influence on the test results.

From the results of the tests, we determined the development path of students N1 and N2. The chemical competency of N1 students increased through tests 1 (3.01), test 2 (3.04), and test 3 (3.28), but the increase was much lower than that of N2 students. The mean score of the tests for N1 students was 3.00, for N2 students was 3.25, and for N2 students was 3.65 (**Figure 6**), this proves that there is an influence of the experimental process on the development of students' chemical competency.

## DISCUSSION

To achieve the goal of teaching and developing students' competencies, the role of the teacher is important. This study surveyed high school chemistry teachers in Vietnam about the problem of teachers using 3D molecular structure simulation in teaching chemistry. The results obtained from 283 survey questionnaires (**Table 6**, **Table 7**, and **Table 8**) show that



**Figure 6.** Students' chemical competency development line (Source: Authors' own elaboration)

most teachers have never used 3D molecular structures in their teaching and a large proportion (44.4%) have never collected 3D molecular structure models and images from open sources on the internet. Statistical results in **Table 6** show that the teaching tools that teachers most often use in teaching organic chemistry are pictures in textbooks (Q1, with a mean of 3.112 being the highest value). In contrast, the use of molecular models created from Q7 software is the least selected option by teachers, and it is also the only option with a mean of  $1.953 < 2.0$  (most of the questions), indicating that teachers' responses are biased towards occasional and never used.  $SD \leq 1$  shows that teachers' choices are relatively consistent.

The results of a survey showed that: teachers have not invested in time or have the skills to exploit and use the source of materials and have not been active in students' learning activities, leading to chemistry teachers not meeting the requirements of the teaching objectives of developing students' competence in teaching in high schools. These are also factors that confirm the research on the causes of difficulties for chemistry teachers in building and using 3D molecular structure simulations in teaching (Q8-Q15, **Table 8**). The most prominent reason is the lack of infrastructures such as the lack of computers, softwareless, or software that needs pay-for-subscription. Teachers claiming that they do not understand the role of simulation is also a cause (Q15). Besides, the lack of skills in using the software was also rated as serious by the teachers themselves (Q14). So that, most teachers only use images of molecular structures from textbooks in class and rarely use 3D molecular structure simulations. This serves as the practical basis for the article's proposal to use 3D molecular structure simulations to develop the chemical competence of Vietnamese students in teaching in high schools.

The teacher's selection of raw materials to be used as teaching aids for 3D molecular structures is consistent with the teachers' confirmations about the extent to which these media are used in teaching about 3D molecular structures organic matter. Thus, the survey

results of 283 chemistry teachers have answered the first research question of the article, which shows that the reality of using 3D molecular structure simulation of chemistry teachers still has many problems that affect the quality of teachers' teaching: The limitations of teachers in using 3D molecular structure simulation in teaching have been pointed out; explore the causes of the limitations in which the main reason is that teachers do not have knowledge about the role of simulation in teaching; The construction and use of 3D molecular structure simulation in teaching are new and difficult for teachers. These are the main reasons affecting the use of 3D molecular structure simulation as well as the teaching quality of Vietnamese chemistry teachers. The teachers' assertions in this article are the practical basis for the research team to propose process of building and using 3D molecular structure models in teaching chemistry. Since then, 16 3D molecular structure simulations have been built to support chemistry teachers' use in teaching (**Appendix B**).

3D molecular structure simulation is a valuable tool to help students understand the structure and properties of molecules. These molecular models can be used to explain the chemical properties of molecules, such as water solubility, solubility in different solvents, and acid-base properties. Besides 3D molecular structure simulation explains the molecular structure and interactions between atoms in the molecule. Compared with students' competency output standards with specific criteria (C1 to C9) (**Table 5**), 3D molecular structure simulation plays an important role in teaching and developing chemistry competence for students. Research assessing the impact of using 3D molecular structure simulation on the development of chemical competence of Vietnamese students.

The survey results confirm that the 3D molecular structure plays an important role in teaching chemistry. 3D molecular structure simulation is a vital tool for explaining the structure and properties of chemical compounds. It helps students understand the chemical nature of substances when participating and forming after the reaction, correctly predict the properties and applications of substances, and apply knowledge to explain the applications of substances in practice and life. In conclusion, using 3D molecular modeling can effectively help develop students' chemistry competence by, as follows:

3D molecular modeling helps students visualize the 3D space of organic substances and hydrocarbons, helping them visualize abstract and complex phenomena. From there, it allows students to interact directly with organic compound molecules, making students better understand the structure and interactions between atoms in the molecule, and the characteristics of each type of hydrocarbon. Through that understand the properties of compounds, including

polarity, solubility in water, boiling point, freezing point, reactivity and applications in life.

Using 3D molecular models encourages students to think scientifically, suggest hypotheses, and test those hypotheses. Students can find new conclusions using 3D molecular models to explain chemical phenomena.

Based on the teaching goals oriented towards the development of students' competency, as outlined by Vietnam Ministry of Education and Training in 2018, and the standard output of students' competency (as outlined in **Table 1**), we built rubrics to assess students' chemical competency in the teaching hydrocarbon section. These rubrics were used to evaluate students three times. Two student groups, out of a total of 630 students, participated in this study. The criteria in the rubrics serve as the basis for us to determine the requirements to be met in the two teaching plans. The highlight of the rubrics is the clarity in the design of the content as well as the criteria for assessing the chemical competence of students before and after the impact on students in groups N1 and N2. Two groups of students were given three tests before the impact, after taking the alkane lesson (2<sup>nd</sup> time), and after studying the alkene lesson (3<sup>rd</sup> time).

The results of the first test (pre-test) were conducted with 630 students. The processing data is indicated in **Table 11**. The mean value of group 1 is 3.01, and group 2 is three. Sig. value between the experimental and control subjects with the first result was  $0.851 > 0.05$ . The results of the pre-test confirmed that the chemical abilities of 630 students who participated in the assessment before the study were similar. Besides the result of the Sig value between gender and the first test result in **Table 10** is 0.877, and between the place of residence and the first test result is 0.141. Both values are greater than 0.05, which indicates that there is no significant correlation between gender and the first test result, and place of residence and the first test result, or no statistically significant difference in students' chemical competence between regions and gender.

The results of tests 2 and 3 showed that, after teachers used 3D molecular structure simulation to teach alkenes, students were given test 2 in which five questions from T21 to T25 have the results of assessing the capacity of these criteria from 3.1 to 3.5 (scale of four) and TN31 to TN35 have results confirming the students' chemical cognitive competency from 3.5 to 3.8 increase compared to the results obtained in test number 1.

Student test results obtained from questions T26 to T28 and T36 to T38 (**Table 11**) are increased from 2.9 to 3.3 and 3.5 to 3.7. This result confirms the improvement of the ability to understand the natural world from a chemical perspective developed through the expression of criteria C6 and C7 (**Table 5**). Understanding the 3D molecular structure of organic compounds can help students visualize complex chemical structures when

represented by visual video. Students can develop critical thinking skills that allow them to apply their knowledge to real-life situations. 3D molecular structure simulation offers an interactive learning experience that engages and encourages students to explore chemistry concepts hands-on. Student test results obtained from questions T29 to T30 and T39 to T40 (**Table 11**) increased from 2.9 to 3.5 and 3.6 to 3.7, confirming the competency development to apply knowledge and skills learned through the expression of criteria C8 and C9 (**Table 5**).

**Table 11** indicates the results of the second test of students' chemical competency. It shows that the influence of building and using 3D molecular structure simulation to develop students' chemical competency in group 2 is greater than in group 1. The data indicates: chemical cognitive competency 1 is formed and developed leading to applying chemical knowledge competency 2 and understanding the natural world from a chemical perspective competency 3 also increases. The results of  $p < 0.05$  in group 2, when compared with  $p > 0.05$  in group 1, confirm the influence of the study on students' chemistry competency. The influence of using 3D molecular structure simulation was further confirmed when looking at the results of the 3rd competency assessment test. Paired samples test statistics show that when comparing values between tests, it shows that the chemical competency of group 2 has a difference in the impact of the study. Sig. values between the subjects and the results of test 2 and test 3 were both  $< 0.05$ , indicating that the subjects correlate with the results of the students' chemical competency assessment, given that the experimental process has an impact on the test results (**Table 12**).

Thus, this study is more general than previous studies that focus on the influence of virtual media such as experimental videos and 3D molecular structure models on the interpretation of the nature of specific substances' structures. It studies the effects of using 3D molecular structures on students' chemical competency in teaching organic chemistry. Dori and Barak (2001) have previously studied and concluded on the influence of 3D molecular structures to explain properties of matter such as molecular structure and physical properties. Additionally, research by Underwood et al. (2021) has shown the influence of understanding molecular structure on understanding the physical properties of substances and the ability to use structure to explain those properties (differences in boiling points of different substances are due to different molecular structures).

This article has elucidated the role of using a 3D molecular structure model in teaching organic chemistry to affect chemical cognitive ability, including the concept of organic compounds, the structure of organic compound molecules, nomenclature and characteristics of chemical bonds, molecular shape in molecules of organic matter, structural formulas of isomers, physical

properties, characteristic chemical properties of compounds, comparison of reactivity, writing chemical equations for the reactions of organic compounds, ability to apply learned knowledge and skills, including applications of substances in practice and methods of preparation in the industry, causes of air pollution, and some measures to limit environmental pollution.

Furthermore, it has been confirmed that studying the influence of modern learning tools such as spatial molecular structure is an effective approach for students to explain molecular dynamics as a chemical concept, or the motion of molecules before and after collision (Casselmann et al., 2021; Guspatni, 2021). The reason, this approach can help students to understand the natural world from a chemical perspective.

The process of using 3D molecular structure simulations, performing tests, and assessing the three components of the chemical capacity completed the research's second objective, answering the second question: "How can 3D molecular structure simulations be used to develop students' chemistry competencies effectively?" The results of this study can be used to guide research into the effects of using 3D molecular structure simulations to study the structure of organic compounds, predict the structure of organic compounds, explain the properties of substances, and further investigate the bonding nature in organic compounds to explain the mechanism of reactions such as the substitution reaction in alkanes (SR), the addition reaction mechanism of electrophiles (AE) in alkene, and the cleavage and bond formation in organic molecules before and after the reaction.

An understanding of the reactive nature of organic molecules is important for manipulating the properties of substances to explain chemical phenomena in real life, which are skills required for chemical competency. Therefore, teachers have achieved the goal of teaching and learning to develop learners' competencies according to the requirements of the 2018 Vietnamese high school curriculum.

The integration of skills to form chemistry competency is consistent and clear. Students in group 2 used 3D molecular structure models to predict and explain the properties and mechanisms of reactions, thereby forming and developing their competency to understand the natural world, and the competency to apply learned knowledge and skills.

The results of assessing students' chemical competency through the use of 3D molecular structure simulation in teaching gave the answer to the research's third question. It is an important tool in chemistry teaching and can effectively help develop the three components of chemistry competence. However, the use of 3D molecular models needs to be combined with linguistic explanations to help students better understand. In addition, attention should be focused on

using 3D molecular models to account for abstract and complex concepts.

According to the article, the use of 3D molecular structure simulations plays a vital role in developing the component abilities of chemical proficiency, as evidenced by the results of tests conducted on 630 students. 3D molecular structure simulations help students to better visualize the structure of chemical compounds, allowing them to understand how atoms and their bonds form compounds and explain their properties. Furthermore, 3D molecular structure simulations develop spatial imagination skills for students. When using a 3D molecular model, students practice spatial imagination by rotating, enlarging, and reducing models. This helps students develop spatial imagination skills, an important skill in chemistry and other scientific fields. Moreover, 3D molecular structure simulations help students develop problem-solving abilities. Students need to analyze the structure of compounds and explain their properties, thereby drawing conclusions about the interactions between atoms and how they affect each other. Therefore, the experimental results have affirmed that 3D molecular structure simulations enhance chemical proficiency for students in teaching chemistry in general and hydrocarbons in particular.

The results confirm that using 3D molecular structure models in teaching chemistry in Vietnamese high schools affects the teaching and development of chemistry competency for students.

### Limitations

The research team has built a solid theoretical and practical basis for their proposals on the impact of using 3D molecular structure simulation in teaching organic chemistry. However, due to the limited time of the research, the background work such as building survey questions, investigating and evaluating the real situation using simulation of the appropriate molecular structure, chemistry teacher's organic materials, determining the goals to be achieved on chemistry competence, designing lesson plans and building rubrics to test and assess competence was done in a school year. Furthermore, the pedagogical experimentation was only conducted in experimental and control classes for five weeks and taught experimentally two teaching plans with four hours of teaching as prescribed. Additionally, the new study only considers the effect of using 3D molecular structure simulation on the development of students' chemical competence in teaching alkane, an alkene, not on alkyne, arene, and compounds organic compounds with other functional groups. Therefore, further studies are needed to explore the role of understanding the molecular structure, thereby studying the relationship of structure to the physical and chemical properties of organic substances. Moreover, understanding molecular structure is the basis for

explaining the nature of substances, for example, the cause of substances with different boiling points is due to different molecular structures (Underwood et al., 2021). This is also the basis for further studies in teaching organic compounds in teaching chemistry in high schools.

## CONCLUSIONS

In summary, using 3D molecular structure simulation to help students study and observe the mechanism of a reaction, particularly focusing on bond cleavage and formation in a compound molecule, has improved their competency in predicting and explaining the properties of substances. Students have then applied the knowledge and skills they have learned to explain chemical phenomena in practice and life. This has demonstrated their skill in constructing explanations, such as being able to identify the characteristics of chemical bonds and molecular shapes in organic molecules, predict physical properties, characterize chemical properties of compounds, compare reactivity, write chemical equations of reactions of organic compounds, perform chemical reactions, and explain the mechanism of the reaction. For example, why bromine is easily substituted in C sp<sup>3</sup> has a higher order, or why the ability to add H-X to C atoms carrying double bonds in alkene molecules with a different number of H atoms is not the same (AE). Thus, students have applied their chemical knowledge to detect and explain some natural phenomena, the application of chemistry in life, and to critique and evaluate the influence of a practical problem. The results of assessing the ability of students in group 2 compared to group 1 through 3 tests have confirmed that using 3D molecular structures is more effective than other interactions such as using models in textbooks to facilitate students' understanding of stereochemistry, a spatially demanding scientific concept (Harle & Towns, 2011). Students in group 2 have a higher chemical competency than group 1 and this competency is increased through the stages before impact, between impact, and after impact. Chemistry competence is demonstrated through students' self-perception of the effectiveness of learning about the molecular structure of organic compounds using 3D molecular structure simulation. Quantitatively, it has been confirmed that students understand the relationship between the 3D molecular structure simulation of organic compounds and their properties and can infer the properties based on parameters in the molecule, such as bond distance and bond angle.

### Implications for Teaching and Future

In recent years, there has been a strong push to rethink the general chemistry curriculum in order to develop students' competencies. Extensive research has shown that students in group 2 go through the same

curriculum as group 1 students, but with the use of 3D molecular structure simulations to study molecular structure and observe and explain the bond breaking and formation of new bonds during chemical reactions, creating products of chemical reactions. This is the basis for students to understand the mechanism of organic chemical reactions. The results of the competency assessment tests (Table 11) confirmed that the students had learned about the molecular structure and the mechanism of the SR substitution reaction of alkane molecules and the addition of AE of alkene molecules, which had a significant impact on their perception of chemistry competency, their ability to apply knowledge and skills, and their understanding of the natural world from a chemical perspective. Moreover, the mean value of chemical competency of students in groups 1 through 3 increased from test 1 (3.01) to test 2 (3.03) and test 3 (3.28). However, the rate of increase was much lower than that of group 2, whose mean value of chemical ability increased from test 1 (3.00) to test 2 (3.24) and test 3 (3.65) (Figure 5). Thus, it is necessary to expand the study of the effects of using 3D molecular structures on the development of students' chemical competency, especially emphasizing the competency to perceive chemistry, including skills such as comparing, classifying, selecting objects, concepts, or chemical processes according to different criteria, and explaining and reasoning about relationships between objects, concepts, or chemical processes (structure-properties, cause-effect, etc.) when studying other hydrocarbons and organic functional groups such as alcohols, aldehydes, ketones, or carboxylic acids, etc.

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## APPENDIX A: GOOGLE FORMS



Form Link: <https://forms.gle/28YwbvRExK8wB6MS6>

## APPENDIX B: QUESTIONNAIRE TO INVESTIGATE THE CURRENT SITUATION OF USING SIMULATION OF MOLECULAR STRUCTURE IN TEACHING CHEMISTRY

**Q1.** Which of the following teaching means do you use to teach the molecular structure of organic compounds? And your frequency level?

**Table B1.**

Content/criteria	Always	Frequently	Occasionally	Never
Pictures in textbook				
Draw into the blackboard or use pictures				
Pictures from the Internet				
The assembled molecular model				
Make models from simple materials				
Virtual models via the Internet, web, etc.				
Molecular model created from computer software				
Self-assess level of using simulation of molecular structure of organic compounds in teaching				

**Q2.** Level of use of the following software for chemical simulation design?

**Table B2.**

Content/criteria	Always	Frequently	Occasionally	Never
Adobe Flash				
Chemical simulation software (Chembio, Chemoffice, Chemwin, ADC Lab, ChemLab, Hyperchem, ObitanViewer)				
Chemistry websites				
Microsoft Office software (Powerpoint, Word, etc.)				

**Q3.** According to you, how effective is use of simulated molecular structures in following forms in teaching chemistry?

**Table B3.**

Content/criteria	Very effective	Effective	Less effective	Inefficient
Ask students to study molecular structure simulation BEFORE class				
Show students a simulation of a chemical molecule's structure IN/WITHIN the class				
Show students a simulation of a chemical molecule's structure AFTER class				
Teachers guide students to build simulations of molecular structures by themselves before learning new lessons				

**Q4.** According to teachers, how important is use of molecular structure simulation in learning process of students?

**Table B4.**

Content/criteria	Very important	Important	Less important	Not important
Create interest in learning chemistry				
Explain molecular structure				
Predict & explain physical properties				
Predict & explain chemical properties				
Overall learning outcomes				

**Q5.** According to you, which of the following causes affect the use of simulation of the molecular structure of organic compounds in teaching? (You can choose more than one option)

- Lack of computer
- Lack of software
- Students do not have access to the internet
- Lack of means and teaching aids
- Teaching aids are not usable
- No time to invest in preparing lessons
- Lack of knowledge and skills in using simulation software
- The role of simulation in teaching organic chemistry is not yet understood
- Assume that using simulation is not necessary

## APPENDIX C: TEST LINKS



Test 1: <https://forms.gle/qThGFR6HmtRr5L776>



Test 2: <https://forms.gle/9bLiWdmK3waGQ7sg6>



Test 3: <https://forms.gle/BeBtgQ62vYyLequX8>

<https://www.ejmste.com>