

Spring 2023

## Impact of Virtual Models on Students' Multilevel Understanding of an Organic Reaction

Eli Martin

Follow this and additional works at: <https://scholarcommons.sc.edu/etd>

 Part of the [Curriculum and Instruction Commons](#)

---

### Recommended Citation

Martin, E.(2023). *Impact of Virtual Models on Students' Multilevel Understanding of an Organic Reaction*. (Doctoral dissertation). Retrieved from <https://scholarcommons.sc.edu/etd/7237>

This Open Access Dissertation is brought to you by Scholar Commons. It has been accepted for inclusion in Theses and Dissertations by an authorized administrator of Scholar Commons. For more information, please contact [digres@mailbox.sc.edu](mailto:digres@mailbox.sc.edu).

IMPACT OF VIRTUAL MODELS ON STUDENTS' MULTILEVEL UNDERSTANDING  
OF AN ORGANIC REACTION

by

Eli Martin

Bachelor of Science  
University of South Carolina, 2005

Master of Teaching  
University of South Carolina, 2006

---

Submitted in Partial Fulfillment of the Requirements

For the Degree of Doctor of Education in

Curriculum and Instruction

College of Education

University of South Carolina

2023

Accepted by:

Hengtao Tang, Major Professor

Lucas Vasconcelos, Committee Member

William Morris, Committee Member

Anna Clifford, Committee Member

Cheryl L. Addy, Interim Vice Provost and Dean of the Graduate School

© Copyright by Eli Martin, 2023  
All Rights Reserved.

## DEDICATION

I would like to dedicate this work to my husband, daughters and parents. Thank you, John, for being supportive of this process. Isabel Mari and Olivia, you have been so patient and understanding. I know the three of you made sacrifices to allow me to complete this process and I am forever grateful. I can only hope that I serve as a strong representation of hard work and dedication to continuing my learning journey as a wife, mother, and instructor. To my parents, Ellie and Luis, you have always been in my corner to push and encourage me through thick and thin- thank you both.

## ACKNOWLEDGEMENTS

I must acknowledge my cheerleader and study buddy in this process, Kat Degar. I cannot imagine having done this without you, your kind words, feedback, and emotional support.

I want to also acknowledge participants of this study. First, you were instrumental but more importantly, and I suspect you are unaware of this, you all were so enthusiastic and encouraging. This meant the world to me. Many of us had already been together at the start of COVID-19 lockdowns and the following difficult transition year from hybrid to “normality.” That you returned for a second year of chemistry was impressive on your end and a compliment. I can only hope that I have made an impact on you, as you have made a permanent impression on me in my learning journey.

I cannot forget Dr. Tang and Dr. Bice. You both provided me with guidance and encouragement to keep me motivated when I was feeling less confident. Thank you for your support.

## ABSTRACT

As the number of STEM opportunities and the need for a scientifically literate society increases, educators in STEM fields require tools that help support these needs. Chemistry is one STEM content area that would benefit from exploring educational technology that supports conceptual understanding. An action research study was conducted to understand how students engage with the content and virtual representation to develop their understanding of a chemical reaction. This convergent mixed methods study looked at the effect of dynamic virtual molecular representation on students' ability to understand a reaction mechanism at the symbolic and subparticulate level by measuring content knowledge and how they verbally explain a mechanism. High school students learned to create virtual molecular models and used the electrostatic potential mapping filter to highlight subparticulate properties. These subparticulate properties, now shown in a dynamic 3D representation, connected students to concepts such as formal charge and electronegativity. These concepts helped students explain if and how two reactants may react in the symbolic model of a reaction mechanism. Qualitative and quantitative data were collected from a pre-post assessment, articulation assessment, and interview. Quantitative data was analyzed using descriptive statistics and Wilcoxon signed rank test, and inductive analysis was used to analyze qualitative data from the interview. Findings indicate that the virtual modeling did support participants understanding of the content, application of concepts to the reaction mechanism and

positively perceived the use of virtual models. In the area of chemical education, the findings in this study are significant because it determined there was an improvement in understanding when students interacted with 3D virtual models but also provided insight as to how participants interacted with the virtual models and the importance of how virtual modeling is embedded into lesson activities.

## TABLE OF CONTENTS

Dedication .....	iii
Acknowledgments.....	iv
Abstract .....	v
List of Tables .....	ix
List of Figures .....	xi
Chapter 1: Introduction .....	1
National Context.....	1
Local Context .....	3
Statement of the Problem .....	4
Statement of Research Subjectivities and Positionality .....	5
Chapter 2: Literature Review.....	11
Introduction.....	11
Chemical Education .....	14
Representational Models.....	20
Reaction Mechanisms .....	26
Cognitive Learning Theory.....	30
Chapter 3: Research Design .....	36
Setting and Participants.....	37
Innovation .....	39



Data Collection .....	52
Data Analysis .....	61
Procedures and Timeline.....	67
Rigor and Trustworthiness.....	72
Plan for Sharing and Communication.....	74
Chapter 4: Analysis and Findings .....	75
Quantitative Analysis and Findings .....	76
Qualitative Findings and Interpretations.....	82
Chapter 5: Results .....	117
Discussion .....	117
Implications.....	125
Limitations .....	128
References.....	131
Appendix A: Pre- and Post-Test .....	157
Appendix B: Interview Questions.....	161
Appendix C: Segments from the Articulation Assessment.....	168

## LIST OF TABLES

Table 2.1 List of Key Search Terms .....	13
Table 3.1 Topics and Practice Covered After MolView Introduction.....	51
Table 3.2 Research Question and Data Source Alignment Table.....	53
Table 3.3 Entry Point Knowledge Assessment and Objectives Table.....	55
Table 3.4 Pre-post assessment and Objectives Table .....	56
Table 3.5 Reactants for the Pre-post assessment .....	56
Table 3.6 Content Related Interview Question and Prompt Alignment to Research Questions.....	58
Table 3.7 Alignment of Interview Questions and Research Question.....	59
Table 3.8 Research Question and Data Source Alignment Table.....	61
Table 3.9 Rubric for Pre-post assessment of Open-Ended Reaction Mechanism Questions.....	62
Table 3.10 Rubric for Content Related Interview Questions.....	63
Table 3.11 Rubric for Content Related Interview Questions.....	64
Table 3.12 Concept Descriptions and Objectives for Student Articulation.....	65
Table 3.13 Stage Description and Timetable.....	67
Table 4.1 Prior Knowledge, Objectives, Mean and Standard Deviation Alignment Table.....	78
Table 4.2 Median Scores for Pre-post assessment Questions.....	79
Table 4.3 Wilcoxon Signed-rank Test Result .....	81
Table 4.4 Mean and Standard Deviation per Criterion.....	82

Table 4.5 Mean and Standard Deviation per Concept .....	82
Table 4.6 Emergent Themes and Categories, Pattern Codes and Data.....	96

## LIST OF FIGURES

Figure 3.1 2D Virtual (symbolic) Versus Dynamic 3D Virtual (symbolic) Representations .....	41
Figure 3.2 Explicit Versus Implied Atoms .....	42
Figure 3.3 Symbolic and Subparticulate Representations of Propanol.....	42
Figure 3.4 Starting Materials for Acid Catalyzed Fischer Esterification.....	49
Figure 3.5 Sequencing of Events for the Study .....	53
Figure 4.1 Screenshot of Delve Process Code Project.....	85
Figure 4.2 Confirming Context of Interviews Using Happy Scribe .....	85
Figure 4.3 Addition of Context in Delve Using Square Brackets.....	88
Figure 4.4 Screenshot of Google Sheet with Initial Data and Codes.....	91
Figure 4.5 Organization of Data, Codes, Categories within Google Sheet .....	92
Figure 4.6 Categories with Pattern Codes were Cut into Strips for Organization.....	93
Figure 4.7 Draft of Color-Coded Themes Done by Grouping Categories.....	94
Figure 4.8 Copies of MS Excel and Google Sheet Spreadsheets .....	95

# CHAPTER 1

## INTRODUCTION

### **National Context**

In the 2018 Program for International Student Assessment (PISA) study, the United States scored statistically lower than 11 international educational systems in science literacy (Sen et al., 2019). A total of 77 other worldwide systems participated. The science literacy assessment encompasses how “students engage in reasoned discourse about science and technology utilizing their knowledge of facts and theories to explain phenomena scientifically” (U.S. Department of Education, 2020). The assessment also requires students to know the standard methodological procedures and patterns of reasoning used in science to evaluate or design scientific inquiries and interpret evidence.

The United States Department of Education defines programs of Science, Technology, Engineering, and Mathematics (STEM) to include skills such as information sense-making, making decisions based on evidence, and using prior knowledge to solve novel problems (U.S. Department of Education Institute of Education Sciences, 2020). Our students need to be strong in these disciplines to be competitive in the world and workforce in which they will be adults. In December 2018, the Committee on STEM Education of the National Science and Technology Council issued a report presenting a five-year plan with a goal that the United States would be a leader in STEM literacy. The Committee on STEM Education of the National Science and Technology Council states that the success of our nation demands a STEM-literate society. To do this, teachers of

STEM subjects need to know how to support students in creating multidimensional and scientifically accurate explanations of abstract concepts using the appropriate resources available for the objective.

When looking at premedical students and engineering students, chemistry courses have been discouraging and a cause for pre-med students to change majors (Rowe, 1983; van Lanen et al., 2000). Organic chemistry, in particular, has been described as a “roadblock” course (Austin et al., 2015). Understanding the concepts in chemistry that students struggle with can help college students avoid changing a major, help improve student confidence in the course at the high school and college level and increase scientific knowledge of the general public.

Gilbert and Treagust (2009) describe three different levels of chemical literacy. The lowest level entails the understanding needed for everyday life to maintain basic needs such as food and shelter. The highest level of chemical literacy, coined as “cultural chemical literacy,” allows one to engage in a conversation with a chemist at a professional level (Shwartz et al., 2006). Chemical education is challenging for many students because of the abstract nature of atoms, molecules, and electrons. Engineering and physics are areas of study in which virtual models can be as effective as concrete models (Klahr et al., 2007; Zacharia & Olympiou, 2011). Compared with the study of chemistry, these fields have different requirements for learning (Stull et al., 2016) and rely heavily on the use of the symbolic level and macroscopic levels of understanding. Organic chemistry, in particular, is highly composed of abstract concepts that must be mentally manipulated (Stull et al., 2013). This is where the study of virtual models in

chemical education is important. How an instructor uses models in an activity to facilitate understanding at different levels of the concept is essential.

Chemistry is complex because students have difficulty explaining a chemical phenomenon because the subparticulate level of understanding must be connected to what is seen (the macroscopic level) by the student along with the symbolic level (math or chemical equations) (Barrett et al., 2015; Gabel, 1998; Gilbert & Treagust, 2009). These difficulties may be overcome with the aid of chemical educational technology, such as virtual representation. The use of educational technology to aid student learning is supported by professional organizations such as the National Science Teachers Association. Virtual models of dangerous chemicals or environments can provide students with experiences that are otherwise not safe. However, to use these resources, the activity, expected outcomes, and tools must be carefully evaluated with the context of the lesson (Barrett et al., 2015; Bongers et al., 2020; Stull & Hegarty, 2016).

### **Local Context**

At all levels of chemistry, students have a difficult time with conceptual and mental models of abstract concepts, such as electrons. In turn, it becomes difficult for students to understand the chemical phenomenon (Bongers et al., 2019), such as the relationship of what is occurring within a reaction and the chemical and physical properties of compounds within the chemical reaction. Using virtual models in programs such as MolView can help students create better mental models (personal models) and more accurate conceptual models that are “coherent and scientifically accepted” representations (Bongers et al., 2019, p. 554).

This state does not provide stand-alone content standards for a high school Organic Chemistry, Pre-organic chemistry, or Chemistry 2 course. The content covered in Chemistry 2 at Bellefield High School (BHS) is the only known program in the state. In other districts in the state, Chemistry 2 is a continuation of Chemistry 1 inorganic content. For some districts, this is in part because Physical Science, a ninth-grade course that covers pre-chemistry, is no longer required curriculum, and therefore, the school no longer offers the course. BHS, at the insistence of its science teachers, continues to highly recommend Physical Science for incoming freshmen. At BHS, Chemistry 2 is allowed to be an expansion of select Chemistry 1 units, including chemical bonding, chemical reactions, and acids base chemistry, and prepares students for organic chemistry by using this prior knowledge.

### **Statement of the Problem**

Students have difficulty explaining concepts in science, in particular chemistry. This can have long term effects for undergraduate students in college and is a reason for STEM undergraduate student majors switching to non-STEM undergraduate programs. A particularly abstract concept is how electrons and atoms interact to predict a chemical reaction. There is work showing that when students can make connections between the submicroscopic level, macroscopic level, and the symbolic level, students have a better understanding of chemical phenomena, such as a chemical reaction mechanism.

### **Purpose Statement**

Students were exposed to concepts and content that many college individuals are not exposed to unless enrolled in an Organic Chemistry course. This exposure widened students' prior knowledge of chemistry. In addition, it exposed students to both the



subparticulate and symbolic levels to develop their own mental models of how molecules interact with each other. This ability has created success in science (Al-Balushi, 2009; Mathewson, 1999; Shepard, 1988; Stieff, Hegarty, & Dixon, 2010; Yair, Schur, & Mintz, 2003). This results of this study suggested a means to support future STEM undergraduate majors, especially those requiring Organic Chemistry or skills required in Organic Chemistry.

The purpose of this action research was to assess how the use of virtual models influenced high school students' ability to accurately understand and explain electron interactions in a chemical reaction using the symbolic and subparticulate representational levels of understanding in a Chemistry 2 Honors course at Bellefield High School.

### **Research Questions**

**RQ1:** How does students' ability to complete a reaction mechanism change after using 3D models to explore the symbolic and subparticulate representational levels of chemistry?

**RQ2:** How do students articulate the process of a reaction mechanism after manipulating 3D virtual models?

**RQ3:** What is the students' perception of using 3D models to learn a chemical reaction?

### **Statement of Research Subjectivities and Positionality**

As an educator, I am always interested in figuring out what is going on in a situation. I try and determine how to help students by listening to their discussions, evaluating the sources of their questions, reviewing their work, and then trying to make improvements to their thought processes as they connect the levels of understanding to

create a bigger picture of the chemistry content. Technology has historically served as a tool to improve measurement, data collection, and functionality, improving an aspect of life. Educational technology now stands to do the same for student performance. A pragmatist paradigm aims to resolve problems by using the available means (Creswell & Creswell, 2018). A pragmatic paradigm for this action research allowed me to evaluate where students were in their conceptual understanding and determine how to proceed to help them make sense of various models, including virtual models, to add to their understanding of a chemical phenomenon.

Over time, I have learned to bristle at the thought of educational technology. It came from how I saw other teachers use it and what I would hear students say about it. For students, I felt like it was an overload but could not make an argument. In all honesty, I am against the use of educational technology in the classroom. Except when

- students have training opportunities without content objectives to meet,
- technology enhances a lesson otherwise not possible,
- technology promotes new thoughts or perspectives, and
- lessons are not based on the technology but on the learning objectives.

In my classes, you can see hints of Herr and Anderson's (2005) “reciprocal collaboration” (p. 31) with my students. This is the positionality I assumed for my research because it benefited the research itself and felt most natural for the students and myself. With a long history of communicating with students about their needs and what I can do to meet them, I believe this came organically to my students and me. This positionality allowed students to feel less observed and more comfortable once the actual

data collection process began. It allowed us to continue with conversations we had already engaged in during other units.

For stakeholders such as school administration, district administration, and parents, my positionality was an insider, having worked in the school and with the district office for over a decade. For parents, this may be the second child whom I taught, and many students are second-year students. Power dynamics were a potential implication of my positionality, in particular with parents and students. While having established rapport with second-year students mitigated this issue, maintaining existing relationships also helped me foster new relationships with the first-year students to minimize power dynamics.

As a new researcher, now studying what I have been trained to do, my biggest concern was the bias I had in my own ability to interpret students' understanding of the studied phenomenon. When consulting with students in class, I verified their thinking process to ensure we were on the same track and spot how misconceptions were being formed. Sometimes I assumed the causes for the misconception or lack of information only to realize 10 minutes later the root of the issue. This situations were mitigated by having other chemistry educators analyze data.

## **Definition of Terms**

### **Virtual Model**

Virtual models will be defined as two-dimensional (2D) or three-dimensional (3D) interactive representations of molecules, electrons, and atoms created by a computer program or application. This is similar to Moyer et al.'s (2002) definition of virtual manipulatives in mathematics, which are described as “interactive, web-based visual representation of a dynamic object that presents opportunities for constructing mathematical knowledge” (p. 373). Stull et al. (2013) and Barrett et al. (2015) define virtual models as 3D interactive computer visualizations.

### **Conceptualize**

The online Cambridge Dictionary defines conceptualization as forming an idea in one's mind (Cambridge Dictionary, 2023). This study uses the term to describe the conglomeration of multiple concepts to communicate a broader idea.

### **Concrete Model**

Models that can be observable at the macroscopic level (Lin et al., 2016) or manipulated by hand and are 3D are considered concrete models. Models of the subparticulate level provide visuals to selected salient conceptual features such as 3D spatial arrangements (Stieff et al., 2016).

### **Two-Dimensional Model**

Two-dimensional models are drawings that are created by hand on paper or by a computer program or application, which lack depth.

### **Three-Dimensional Model**

Examples of 3D models are ball and stick molecular representations built by the student. It will also include those created by a computer program or app that allow for rotation and manipulation. This manipulation may occur on a touch screen or by using the computer's mouse pad. To be considered three-dimensional, the image must have the appearance of depth.

### **Conceptual Model**

These are models that have been deemed scientifically accurate to explain salient features of a concept (Bongers et al., 2019).

### **Mental Model**

Mental models are representations of an idea or object created by the imagination which cannot be observed (Bongers et al., 2019; Chittleborough & Treagust, 2007; Johnstone, 1993). Mental models can be made visible by asking one to draw or create a visual representation of their model.

### **Symbolic Level of Understanding**

The symbolic level in chemistry is made up of chemical symbols, chemical formulas, balanced or skeletal chemical equations (Gilbert & Treagust, 2009). Johnstone (2000) and Gabel and Bunce (1994) interpret the symbolic as expressions to communicate information. Others describe it more broadly to include graphs, reaction mechanisms, algebraic, and computational forms (Kozma & Russell, 1997; Russell et al., 1997; Treagust et al., 2003). I define the symbolic level methods of communicating chemical information that includes models, diagrams, formulas, and graphs.

### **Subparticulate Level of Understanding**

The term “subparticulate” is often interchanged with the microscopic or particulate level. Regardless of the name used, they all intend to describe matter that we cannot see. Sometimes it can be seen with a visual aid such as a microscope. Other times, these terms refer to abstract concepts such as electron movement and are described through pictures or other types of models. Johnstone (1982) originally labeled this level as explanatory. It communicates the theory behind concepts observed and represented through symbols. Bucat and Mocerino (2009) further describe the subparticulate level in chemistry as “an unobservable world, accessible only by imagination (p. 12). For the purpose of this work, the term subparticulate is used to emphasize that electrons and atoms cannot be seen.

### **Macroscopic Level of Understanding**

Macroscopic phenomenon or models are visible to the student. They may include chemical or physical properties such as flammability and color. Simply stated, macroscopic is defined as an “observable phenomenon” (Creswell & Creswell, 2018).

## CHAPTER 2

### LITERATURE REVIEW

#### **Introduction**

Chemistry education often incorporates three levels of understanding, the macroscopic, subparticulate, and symbolic (Gilbert & Treagust, 2009; Johnstone, 1982; Taber, 2013; Talanquer, 2011). While the names and number of levels may vary in the literature, it is known that it is difficult for chemistry students to master all three levels to explain a particular chemistry phenomenon (Chandrasegaran et al., 2009; Gabel & Bunce, 1994; Keiner & Graulich, 2019; Trivic & Milanovic, 2018). Work shows that when students can make connections between the subparticulate level, macroscopic level, and the symbolic level, students have a better understanding of chemical phenomenon (Bongers et al., 2020; Gkitzia et al., 2019; Ye et al., 2018) such as a chemical reaction. With the availability of educational technology in the field of chemistry education (Bongers et al., 2020; Cai et al., 2014) combined with careful scaffolding (Harris, 2019; Stieff et al., 2011; Wang & Barrow, 2011; Williams & Clement, 2015) there is an opportunity to improve students' understanding of chemistry at two or three levels of understanding and potentially increase and maintain students' interest in this field.

The purpose of this action research was to assess how the use of MolView virtual models influence high school students' ability to use two of three levels of representational understanding (the symbolic and subparticulate) to accurately explain

a chemical reaction as they attended a Chemistry 2 Honors course at Bellefield High School. The research questions to guide this work were

**RQ1:** How does students' ability to complete a reaction mechanism change after using 3D models to explore the symbolic and subparticulate representational levels of chemistry?

**RQ2:** How do students articulate the process of a reaction mechanism after manipulating 3D virtual models?

**RQ3:** What is the students' perception of using 3D models to learn a chemical reaction?

To guide the literature review to these questions, the following variables were pulled from the research questions: (a) representations in chemistry, (b) virtual representation, (c) concrete modeling, and (d) reaction mechanisms or, more broadly, chemistry education. To further investigate the topic of science learning with models and modeling, an additional search into CLT, cognitive load, and dual coding was conducted.

Key terms used to conduct this search varied depending on the chemistry context or framework. Overall, the most common terms used were chemistry education, educational technology, models, organic chemistry, and science education. The search started very broadly but did narrow down when using key terms found within research studies. The process of narrowing down key terms was done by substituting common phrases and using key terms from valuable resources. Another strategy was using quotation marks, although, at times, this narrowed down the content too much and in the wrong direction. For example, reaction mechanism and science education often produced results from medical training research. Changing science education to "chemistry



education," adding the term secondary education and using quotations around reaction mechanism produced better results. The following is the complete list of terms used.

Table 2.1 List of Key Search Terms

"chemistry education"	Chemistry education research	Language	Science education
"reaction mechanism"	Cognitive learning	Mental rotation	Secondary science
"Chemistry education"	Cognitive learning theory	Modeling	Spatial ability
"Computer model"	Cognitive load	Models	Spatial development
"Virtual model"	Cognitive load theory	multimedia learning theory	Spatial skill
2D model	Conceptualization	Multiple levels of understanding	Spatial training
3D model	Concrete modeling	Multiple representations	Static representation
3D model or representation	Concrete models	Multiple representations in chemistry	"student explanation"
Action research	congruity	Organic chemistry	Student performance
Augmented reality	Difficulty	Performance	Teaching chemistry
Chemical education	Dual coding	Representational levels	Think aloud
Chemical education technology	Dynamic representation	Representational translation	Understanding
Chemical reactions	Education	Science	chemical reactions
Chemistry	Educational technology		Virtual model
Chemistry education	Fluency		Virtual modeling
	High school chemistry		Virtual models
	Instructional methods		Virtual representations
			Visualization

Sources used to conduct these searches include *ERIC*, *EBSCO*, *ProQuest*, *ProQuest USC*, *Google Scholar*, *Education Source database*, *Royal Society of Chemistry*, *Chemical Education Research and Practice*, and *American Chemical Society*. This literature review will discuss the following topics:

1. Chemical education and its definition and requirements for understanding.
2. Levels of understanding chemistry and the (a) macroscopic, (b) subparticulate and, (c) symbolic.
3. Challenges within chemical education

4. Chemical educational technology and its usage
5. Representational models and (a) scientific representational models, (b) models and instructional strategies, (c) models in chemistry, (d) symbolic understanding and its representational models, (e) macroscopic understanding and its representational models, (f) subparticulate understanding and its representational models and finally, (g) representational models to connect the subparticulate and symbolic levels.
6. Reaction mechanisms and their (a) importance and (b) current research.
7. Conceptual framework and (a) cognitive load theory, (b) working memory and long-term memory, (c) intrinsic and extraneous cognitive load, (d) cognitive load and, (e) dual coding.

### **Chemical Education**

This section will define chemical education, levels of understanding chemical education, and discuss the challenges teachers and students encounter.

#### **Defining Chemical Education**

Chemical education has been changing. As the studies in technology, biology, materials, energy, physics, and medicine grow, their connection to chemistry becomes more apparent (Mahaffy, 2015; Pearce, 2002). There is a movement to redesign undergraduate-level chemistry courses to reflect their cross-curricular nature. This is encouraged by emerging research in chemistry and chemistry degree holders (Pearce, 2002). Chemical education and chemistry education are becoming two separate modes of thinking and teaching chemistry (Mahaffy, 2015). Chemistry education does not isolate its content from human activity. Context is a required pedagogical practice in chemistry

education. Chemical education, on the other hand, is stand-alone content. This study was limited to chemical education.

When we look at chemistry in isolation, it is the study of matter, its components, periodicity of properties in matter, energy, and types of chemical reactions (Gilbert & Treagust, 2009). Connecting these macroscopic and symbolic components is a language unique to chemistry, entailing a synthesis of representative models depicting electrons, atoms, molecules, and such (Nahum et al., 2004). It considers the subparticulate and macroscopic components and theorizes as to their behavior and appearance (Jaber & BouJaoude, 2012). Models, laws, and theories are used as tools to predict and explain the macroscopic level (National Academy of Sciences, 2013). Understanding and communicating chemistry at any degree requires “mentally engaging with representations” (Gilbert & Treagust, 2009, p.3) to connect the macroscopic, symbolic, and subparticulate levels. Experts fluently move between the macroscopic, symbolic, and subparticulate levels to communicate information (Johnstone, 1991, 1993; Kozma, 2003; Kozma & Russell, 1997; Taber, 2013). This language is part of the education of chemistry (Childs et al., 2015; Corradi et al., 2012; Kermack & Robinson, 1922; Kozma & Russell, 1997). While the definition of chemical education is changing, I argue that some traditional facets cannot be avoided, including its language.

### **Levels of Understanding Chemistry**

In this section, the following will be discussed by first defining the (a) macroscopic, (b) subparticulate, and finally, (c) symbolic levels.

Gabel (1993) refined Johnstone's (1982) ideas of forms of chemistry as three levels of teaching chemistry or levels of understanding chemistry. Coined the triplet by

Talanquer (2011), these levels of understanding chemistry came from Johnstone's essay in 1982. While the levels of understanding are helpful individually, students of all ages have difficulty translating between and connecting the levels (Johnstone, 2000). These levels include the macroscopic, subparticulate, and representational (symbolic).

The *macroscopic level*, sometimes described as phenomenological (Gilbert & Treagust, 2009) describes properties that often can be seen and quantified or qualified with the senses or available tools (Gilbert et al., 2000; Gilbert & Treagust, 2009; Johnstone, 1982). These properties may include color, mass, and other physical or chemical properties. The macroscopic level is observable. What is observable has changed as technology improves, in turn changing the term. Traditionally, what we cannot see is labeled as the subparticulate or microscopic level (Gilbert et al., 2000; Gilbert & Treagust, 2009; Johnstone, 1982). Here it is termed subparticulate.

The *subparticulate level* entails abstract concepts such as atoms, molecules, and electrons. More simply, it is what we cannot see (Gilbert & Treagust, 2009). However, with technology such as scanning tunneling microscopy, scientists can see the atomic level and beyond (Cang et al., 2008), blurring the line between what has been traditionally classified as macroscopic and subparticulate. Technological advancements have allowed humans to experience the subparticulate level making terms, such as macroscopic, obsolete (Talanquer, 2007). What occurs at this level is how we explain what we see (Gilbert & Treagust, 2009). Gilbert and Treagust (2009) define the subparticulate level in chemistry as "an unobservable world, accessible only by imagination" (p. 12).

The *symbolic level* in chemistry is made up of chemical symbols, chemical formulas, balanced or skeletal chemical equations (Gilbert & Treagust, 2009). Johnstone (2000) and Gabel and Bunce (1994) interpret the symbolic as a means to communicate information. Others describe it more broadly, including graphs, reaction mechanisms, algebraic, and computational forms (Kozma & Russell, 1997; Russell et al., 1997; Treagust et al., 2003). Both definitions of what the symbolic level entails communicate information about the macroscopic or subparticulate world.

### **Challenges within Chemical Education**

While education in chemistry progresses, it still holds onto tradition (Söderqvist, 1997). Chemical education comes with challenges from many fronts (Gabel, 1999). Chemistry is complicated (Johnstone, 1991; Nakhleh, 1992; Taber, 2002) as it is not only abstract in nature but also requires judgment in evaluating plausible explanations (Atkins, 2015). Then, the discussion of chemical phenomena requires its own vocabulary and language (Gilbert & Afonso, 2015). The first lesson of a chemistry course is when acquiring this language begins (Stieff et al., 2011). Not only does the first lesson require absorbing the language immediately, but it requires fluency between modes of representations (Stieff et al., 2011) and the language expressing these representations. To add to this, educators use the language in a course but do not explain how the macroscopic, symbolic, and subparticulate levels are connected to each other (Gabel, 1999). It cannot be taken for granted that students can connect the three levels of understanding. Teachers often neglect to consider students' thinking and reasoning, missing the evolution of students' reasoning and educational practices (Weinrich & Talanquer, 2016). All of this can be overwhelming. Conscious educators may make use

of pre-and post-assessments as an indicator of progress. Unfortunately, a post-test may indicate improved learning performance but does not necessarily mean students can make connections between the three levels or apply them to an observed phenomenon (Treagust & Chittleborough, 2001). This language, described as "mental gymnastics" (Johnstone, 1982, p. 377), is not readily understood by novices (Treagust & Chittleborough, 2001). To aid these challenges, educators can employ chemical educational technology to develop instruction.

### **Chemical Educational Technology**

This next section entails information on (a) educational technology for chemistry, (b) virtual representational models, and (c) limitations.

Chemical educational technology is technology (web-based, simulations, applications, software) that at its core supports the understanding of chemical concepts when used correctly (Al-Balushi & Coll, 2013; Antonoglou & Sigalas, 2011; Barrett et al., 2015; Stull et al., 2013). For example, for safety and feasibility, virtual laboratories are used to simulate experiments. Ideally, information and communication technologies make these simulations as accurate as possible (Martinez-Jimenez et al., 2003). Chemical educational technology is digital technology to enhance education in chemistry, including communication, data collection, representation of concepts, and more.

Students do perceive value in educational technology (Rogers, 2012). A virtual reality (VR) study conducted by Edwards et al. (2019) observed students were engaged and enjoyed the immersive activity even with setbacks such as dropping atoms or molecules obstructing navigation. Lim et al.'s (2018) study on stereochemistry using augmented reality produced responses such as "I feel more aware of the actual molecular

structure than the paperwork, which makes the molecule more impressive" (p. 10).

Clickers and now Next Generation Clickers, which allow instructors to create questions, import and manipulate molecular structures, have shown positive results in performance and perception. (Shea, 2016) notes students' appreciation for the immediate feedback creating engagement between students and students and instructor. The Next Generation Clickers, used in Smith College, also allowed students to assess their own misconceptions in understanding.

Some chemical educational technology serves to create instructional representational models meant to portray different perspectives in chemistry, the macroscopic, subparticulate, and symbolic. These may be 3D, 2D, static, or dynamic. The 3D representations (virtual or print) have the illusion of depth (Merriam-Webster, n.d.). Barrett et al. (2015), Moyer et al. (2002), and Stull et al. (2013) all include features such as interactivity and computer, or web-based generated models. These may be dynamic or animated but do not necessarily permit student manipulation such as rotation or play-back.

Two-dimensional virtual models are web-based images, visualizations, or representation models that lack depth (Merriam-Webster., n.d.). The student may create these models using a touch screen, mouse pad, or other input. These are often static and cannot be manipulated by students to see different perspectives. Two-dimensional virtual representational models often depict the subparticulate and symbolic levels of chemistry.

For abstract and complex processes, there is evidence indicating dynamic representation is superior (Bodemer et al., 2004; Williamson & Abraham, 1995) and evidence that this type of representation is not more effective than static (Yang et al.,

2018). When static and dynamic representations are compared, it has been found that the extraneous information within dynamic representations is more complicated than static representations (Jones, 2013; Jones et al., 2005; Suits, 2015; Suits & Sanger, 2013).

Instructors may use virtual representational models in a way that does not enhance learning and may even inhibit student understanding (Clark & Lyons, 2011).

When educational technology is used for representational purposes, proper selection of dynamic representations can reduce cognitive load compared to static images. However, students may not perceive dynamic representations as less taxing (Yang et al., 2018). Aldahmash and Abraham (2009), Antonoglou and Sigalas (2011), Starbek et al. (2010), and Yang et al. (2018) all indicate the superiority of dynamic representation. Starbek et al. (2010) found little difference between dynamic and static representational model groups. The dynamic and static representation groups did perform better than the other two groups that only used traditional lectures or text.

In Yang et al. (2018), the assessment type proved to be the indicator of superiority. For example, no significant difference was seen on multiple-choice assessments when comparing a group using dynamic representations to one using static representations. The group exposed to dynamic representation outperformed students exposed to static representations on open-ended questions.

### **Representational Models**

Next, I will cover (a) scientific models, (b) models and instructional strategies and, (c) models used in chemistry. This section concludes with examples of representational models used for each perspective of chemistry, the symbolic, macroscopic, and the subparticulate level.



## **Scientific Representational Models**

Scientific models are intertwined with scientific development that the epistemology of one is essential to the epistemology of the other (Akerson et al., 2011; Lederman, 2007; National Research Council, 1996, 2007). The United States Next Generation Science Standards (NGSS) describes elements of the nature of science (NOS) that should be directly taught and addressed in the classroom. One element of NOS is the use of "science models, laws, mechanisms, and theories [to] explain natural phenomena" (National Academy of Sciences, 2013, p. 4). Understanding the NOS and conceptual learning go hand in hand. The more sophisticated the understanding of the NOS, the more improvement in conceptual learning (Clough, 2006; Deng et al., 2011; Kim & Irving, 2009; Songer & Linn, 1991). While models are used to represent accepted abstract and theoretical concepts, they are not complete or accurate representations of these concepts (Caviglioli, 2019; Taber, 2015). Instead, their function is to communicate and predict processes in science (Grünkorn et al., 2014; Krell et al., 2014; Schwarz et al., 2009; Oh & Oh, 2011).

Representational models include diverse types of virtual models but also include concrete or pictorial models. Students can manipulate 3D concrete models through hands-on experiences. Barrett et al. (2015) describe concrete media as a tangible form meant to depict concepts that cannot be seen readily or are abstract in nature. Molecular modeling kits are examples of concrete media that make atoms, bonds, and molecules tangible for students as they build the structure. Other models include 2D and virtual models (static or dynamic), which fall in the category of instructional graphics. Instructional graphics are defined by Clark and Lyons (2011) as visuals, graphics, pictures, and illustrations that

may have inaccuracies but are still intended to enhance student learning. This aligns with their intended use in the NOS (National Research Council, 2007, 2012). When used correctly, using various representational models can benefit learning in chemistry (Patron, 2017). The results on which type and combination of representations are best has not been settled.

### **Representational Models and Instructional Strategies**

Conceptual understanding of representational models as a part of the NOS can be influenced by instructional strategies shifting students' understanding towards or away from scientifically accepted theories. Instructors may select representations based on (a) how useful it appears (Clark & Lyons, 2011), (b) perceiving it to be self-explanatory (van Driel & Verloop, 1999) (c) an effort to match learning styles (Patron, 2017) or (d) a lack of understanding the function of the model (van Driel & Verloop, 1999). All contribute in negative ways. Due to less than ideal instructional conditions, a naïve understanding is developed from a constructivist framework in which the learner forms the misconception that the model is the phenomenon (Grosslight et al., 1991; Krell et al., 2014). This is unfortunate as misconceptions and misunderstanding representational models will lead to inferior performance.

Students do not understand complex concepts simply because models are incorporated within text and activities. Instructors need to incorporate within the lesson how to read the representational model for effective execution (Clark & Lyons, 2004) on identifying salient and irrelevant features. In one study by Rankin (1989), it was found that the overwhelming majority of errors on a comprehension assessment were related to the graphics, while seven percent were due to lack of content comprehension. Two of the

four causes identified by Rankin were unfamiliarity with the representational convention and misinterpretation of the layout. When using dynamic representational models, the same issues arise, encouraging misconceptions (Kelly et al., 2017; Lowe, 2004; Tasker & Dalton, 2008). Before instruction of the representational models is provided by identifying salient features and limitations, the type of model for the lesson must be evaluated.

When selecting the type of symbolic representation, instructors need to account for features that may distract from the focus of the content. In the case of virtual dynamic and static representations, they should not distract or take up more cognitive load in working memory when students are engaging with the representations (Clark & Lyons, 2011). The representational models for this study are meant to activate prior knowledge and minimize the cognitive load by using a web-based application to limit unrelated features, as described by Clark and Lyons (2011).

The lesson's content should guide representational model selection and usage (Barrett et al., 2015). In Mayer et al. (2005), students using dynamic models did as well or more poorly than those using static models. In this case, the lessons were on how brakes, lighting, toilets, or waves work, and the students could not pause and replay the dynamic representations of the lesson. Dynamic representations work better when the goal is to teach a skill and less so when it is a process (Clark & Lyons, 2011). The type of content or expertise required from the lesson objectives will indicate the type of dynamic representation to use.

Concrete representational models can be superior to virtual representational models. Virtual models may require more cognitive effort on the student, taking away

from the lesson's objectives even though both are meant to satisfy the same objective (Fjeld et al., 2007). There is the belief that how concrete or virtual models are used within instruction explains the inconsistencies in effectiveness (Al-Balushi & Al-Hajri, 2014; Stieff et al., 2005; Stull et al., 2013; Stull & Hegarty, 2016).

### **Traditional Models in Chemistry**

Representational models are a dominant feature in chemistry (Nahum et al., 2004). Concrete representations, such as molecular models that the student builds, represent abstract concepts, although they still hold some inaccuracies (Barrett et al., 2015). These representations provide students an avenue to view and manipulate what cannot be seen in the classroom.

Other models used in chemistry are Lewis dot structures, space-filling, or dash and wedge models. These are classified as interpretive graphics as they are symbols used to communicate how the subparticulate level functions as line drawings (Clark & Lyons, 2011). A strength of these models includes that they are used to represent molecular structures, angles, including connectivity between atoms and rotations within molecules (Ainsworth, 2008; Harrison & Treagust, 1996). The drawings come from the student and help expose their thinking of a concept that may be missed in a verbal explanation (Fiorella & Zhang, 2018). Fiorella and Zhang (2018) explain that these drawings present student perception of spatial relationships and abstract features that would also not be noted in other representations such as concept maps. A limitation is that students may believe they are actual representations of the abstract particles they represent and lose perspective in size (Ainsworth, 2008; Harrison & Treagust, 1996).

## **Representation of the Symbolic Perspective**

The language of chemistry is represented with symbolic representations such as chemical symbols, formulas, equations, graphs, and pie charts. Symbols often communicate the structure, properties of atoms, molecules, or reactions (Bongers et al., 2019). The purpose of graphs and charts is to present quantitative information (Clark & Lyons, 2011; Nakhleh & Krajcik, 1994). This type of model is termed relational by Clark and Lyons (2011), and its categorization within scientific models varies (Johnstone, 1991; Nakhleh & Krajcik, 1994; Treagust et al., 2003), complicating the discussion of chemical education (Gilbert & Treagust, 2009).

## **Representation of the Macroscopic Perspective**

Macroscopic representational models reflect the phenomenon. These representations include laboratory, real-life experiences (Treagust et al., 2003) or images of the event (Gkitzia et al., 2019). Virtually created representational models of the macroscopic level of chemistry may be dynamic and allow students to control variables. From macroscopic representations, one can collect information such as mass, color, pH levels, or density from what is observed, compiled into data tables or graphs. The macroscopic level can be linked to the symbolic by collecting real-time data, such as measuring pressure and volume as the plunger of a syringe is manipulated by the student, revealing the inverse relationship between the two variables. Before and after static images of a phenomenon can also be used to prompt discussion. Either way, these representations require explanations at the subparticulate level and the symbolic level to be truly understood.

## **Representation of the Subparticulate Perspective**

Representational models, whether dynamic, static, or concrete, depict molecules, atoms, electrons to help create conceptual understanding. Many may be familiar with molecular models that allow students to build molecules. These concrete models often include links to represent single, double, or triple bonds between atoms. As links are added between two atoms, the geometry around the atom changes reflecting theory on molecular structure. It is prevalent for the change in shape due to bonded and unbonded electrons to go completely unnoticed by students without direct instruction or prompting by the instructor in a high school chemistry class. These subparticulate representations make the invisible visible. Unfortunately, a side effect is that size and perspective may be misconstrued by or remain oblivious to learners.

Next, I will discuss the importance of understanding a reaction mechanism and current research on reaction mechanisms and representational translation.

### **Reaction Mechanism**

Reaction mechanisms are a type of symbolic representation showing the flow of electrons (called electron-pushing formalism or EPF) (Bongers et al., 2019) between reactants of a chemical reaction. In addition to using electron pushing formalism, reaction mechanisms differ from a chemical equation as mechanisms show intermediate molecular structures formed during the reaction.

### **Significance of Understanding Reaction Mechanisms**

Stemming from Christopher Ingold's research and teachings in organic chemistry in the 1930's, reaction mechanisms are taught to demonstrate how and why reactions occur as a means of prediction (Weeks, 1967; Wentland, 1994). While the value of

reaction mechanisms has been argued (Bhattacharyya & Bodner, 2005), its common use in undergraduate organic courses and textbooks is unavoidable (Penn & Al-Shammari, 2008), making reaction mechanisms an integral part of understanding organic chemistry (Bhattacharyya & Bodner, 2005; Bowman et al., 2007; Penn & Al-Shammari, 2008).

For me, the opening statement in Kelly et al. (2017) confirms how students have been taught and the importance of grasping how a student understands chemical concepts.

We are not taught to ask questions. We are taught to learn it and do well on tests, rather than understand it...Everything is always given to you. This is what is happening..., but we don't know why.—S10" (Kelly et al., 2017).

When students can complete reaction mechanisms, there is evidence that these students have less difficulty working with novel problems (Grove et al., 2012). Factors affecting success can vary, so assessment and instructional tools should be considered when designing the instruction.

### **Current Research in Chemical Education**

The next section provided current research on assessment methods in chemistry courses, students approach to solving reaction mechanisms and students' usage of multiple levels of understanding.

Oral assessments are one approach to assess students' understanding. Bhattacharyya and Bodner (2005) noted students' ability to work through a reaction mechanism accurately but were unsuccessful in explaining the process. In this phenomenographical study, 14 graduate students (one with an M.S. in Chemistry) were given an oral assessment of their strategy using the think-aloud protocol (Ericsson &

Simon, 1984). In Webber and Flynn's (2018) grounded theory study, they conducted an oral assessment of students from a redesigned Organic Chemistry II course to gather information on students' thought processes for solving familiar and unfamiliar questions. Here, Webber and Flynn (2018) noticed that intrinsic motivation to try again when the student detected an error during an oral assessment improved student performance. Bongers et al. (2020) also used a think-aloud in a mixed methods study to assess the effectiveness of dynamic representations in students understanding of reaction mechanisms.

Flynn and Featherstone (2017) examined responses resulting from prompts by students to evaluate how students approached reaction mechanisms, noting that how students developed the responses was lacking. Trends in misconceptions and strategies were revealed through the developed coding system. In Bhattacharyya and Bodner (2005), it was found that the reaction mechanism was approached as a puzzle, a strategy I have seen myself.

Familiarity with the reaction was accounted for in Grove et al. (2012) and Webber and Flynn (2018). Students in the Grove et al. (2012) study could transfer knowledge gained in one setting to another. This group of second-year organic chemistry students was asked to predict the products of a chemical reaction and provide the reaction mechanism. This occurred near the end of their course using OrganicPad, a tablet PC program for drawing structures. Parts of the reaction problem were novel and required applying concepts, while other parts were similar to the lecture or textbook materials. The novel component of the assessment makes it more difficult for students to use a puzzle or pattern-like approach. Flynn and Featherstone (2017) took a similar approach by



introducing the content first, then the assessment, followed by the reaction and its symbolism.

The mixed methods study by Gkitzia et al. (2019) on translating between the three levels of understanding revealed difficulties when students translate between the symbolic and subparticulate levels. Students scored better when translating between the macroscopic and subparticulate levels. These quantitative data came from a matching exercise. Gkitzia et al. (2019) also saw that students failed to account for multiple variables in a single representation of a subparticulate level model when translating it to the macroscopic level. They did not know what features of a solid-state of matter model to focus on (Gkitzia et al., 2019). Flynn and Featherstone (2017) noted that students interpret the same molecule shown in two different conformations (symbolic representations) as if the molecules were different. In this study, participants had higher performance rates when the line-angle drawings (symbolic representation) for a reaction mechanism included explicit atoms. This means that the carbons were drawn into the line-angle structure. It is implied that carbons are located on the angles and ends of the line accompanied by hydrogen atoms. Atoms that are not carbon or hydrogen are explicit in line-angle drawings.

These studies show that practiced and novel open-ended questions reveal gaps in students' thinking process. Pre-and post-assessments serve as a baseline and can provide insight on translation between representational models.

## **Cognitive Learning Theory**

Cognitive learning theory (CLT) is a theory stemming as far back as 1920 (Bergel, 1998), accounting for learning that takes place over time, with practice, reinforcement allowing the student to reorganize new with existing cognitive structures (Good & Brophy, 1990). Key components include (a) information processing (b) schema theory (c) cognitive load theory, and finally, (d) dual coding theory, which are discussed in the sections below.

### **Information Processing**

Atkinson and Shiffrin (1968) originally proposed information processing models that are still widely used (Driscoll, 2005). Information must move through three stages, each requiring direct and indirect interaction with the individual. Driscoll (2005) describes factors such as attention, pattern recognition and encoding as influencing factors that move information from sensory memory, working memory and to long-term memory. We take in a large amount of information from our senses that is held for a very short amount of time and is lost unless we can recognize patterns and pay attention (Driscoll, 2005). Information that does progress to the working memory stage is held for a very brief amount of time (Baddeley, 2000; Barouillet & Camos, 2007; Cowan, 1995; Miller, 1956) around 20-30 seconds (Driscoll, 2005) holding limited amount of information (Driscoll, 2005; Miller, 1956). For the information to become retrievable, it must next move into the long-term memory. De Groot (1965) and Chase and Simon (1973) found that this information comes from chronic exposure to domain-specific knowledge. Once these constructed pieces of information are in long-term memory, they can then be pulled into working memory for use. At this time, the learner has in their working memory new

information and old information. For the new information to be 'learned,' it must be integrated with what we already know (Sweller,1994). During this integration process, there are events that can inhibit integration (Rop et al., 2018). Avoiding these hinderances moves information to long-term memory where it can be later retrieved.

### **Schema Theory**

The idea of flexible organized frameworks of memories, schemata, did not take root until the 1970 amongst cognitive researchers (Gagne, 1985; McVee et al., 2005; Richey et al., 2011). Considered the atom of cognition (Rumelhart, 1980), these constructed cognitive systems help us retain and recall information (Anderson, 2013) and our understanding of Learning, Design and Technology is influenced by these structures (Neumann & Kopcha, 2018). Sweller et al. (1998) and Jung et al. (2022) state that modifying prior or developing new schema is done best by connecting it to well established schema that does not require much thought from the student. Instructional strategies that begin with activating students' prior knowledge are making use of these cognitive storage systems, which are important for science literacy, and science reading and comprehension (Wright et al., 2016). Imagery and concept mapping strategies have been used by instructional designers (Neumann & Kopcha, 2018) as strategies to develop and modify schemata when new information is presented (Rumelhart & Norman,1978) to an attentive individual. West et al. (1991) and Winn (2004) demonstrated that students can create mental representations encoded from realistic models requiring task recall and manipulation which supports Abel and Kulhavy (1989) study demonstrating that one can effectively take in, or encode, text and imagery together. When accounting for prior knowledge, Hannafin and Rieber, (1989) found that a larger knowledge base increases

encoding and retrieval success rates. All of this is to say that new text, imagery, and prior knowledge all mingle with established schemata to learn new information (Fleming, 1987; Kulhavy et al., 1993; Winn, 1989).

### **Cognitive Load**

Cognitive load theory explains the process of learning requiring the movement of information from working memory into long-term memory (Sweller, 2020). There are factors that can facilitate and hinder this process. Effective instructional strategies account for these factors by maximizing working memory and reducing the cognitive load on working memory (Kirschner et al., 2018).

There are three types of cognitive load placed on working memory. Choi et al. (2014) and Kalyuga (2011) only consider two, intrinsic and extraneous load. They state that the ties between germane and intrinsic make it challenging to distinguish one from the other. Only these will be considered in this study. Working memory uses different types of cognitive load during instruction. A task with many components that are unrelated to what is to be learned, unrelated images, or sound effects will tax working memory. This type of load caused by distracting or irrelevant features is termed extraneous cognitive load (Chen et al., 2017). The learning materials and environment can inhibit the learning process regardless of intention. This is why for this study, evaluating the representational model, how they are presented, exposure to them were all factors to consider as these are components of instruction that can increase the extraneous cognitive load (Brünken et al., 2003; Paas et al., 2003).

Intrinsic cognitive load, on the other hand, comes from the content itself. The nature of the content in this study was complex, which will tax the intrinsic cognitive

load of working memory (Kirschner et al., 2018; Sweller et al., 2011). To create room for intrinsic load, instructional strategies can be used to decrease extraneous cognitive load. (Sweller et al., 2011).

In Johnstone's (1982) essay, he discussed how novice and expert chemistry students should make sense of chemistry at three levels to improve conceptualization in education. More important to him was the need to incorporate a psychological approach and the learning process (Johnstone, 1989, 1991). Cognitive load is one factor to account for in chemical education. Numerous factors can influence cognitive load. For example, each student will have a different working memory capacity (Permana et al., 2019) and domain-specific prior knowledge (Clark & Lyon, 2011). In science education, Meissner and Bogner (2013) suggest reducing cognitive load by factoring into instructional design the (a) task structure, (b) task difficulty, and (c) levels of detailed explanations.

### **Dual Coding**

Dual coding refers to the process of absorbing information from audio and visual components simultaneously (Kirschner, 2019). Instructors should be aware that different modes of representation are absorbed differently (Corradi et al., 2012). Using the two systems, audio and visual, to present the same concepts opens working memory (Kirschner, 2019). Working memory is more effectively used when a visual representation is accompanied by verbal instruction (Caviglioli, 2019). In turn, the experience amplifies the likelihood of retrieving the presented concepts from long-term memory (Caviglioli, 2019). The idea is that dual sources for the same information help solidification within long-term memory. From dual coding, we know when presenting

new information, it needs to be carefully unwrapped to reveal more essential features first (Caviglioli, 2019).

Reducing cognitive load may be done with verbal or text instruction that is clear and concise (Mayer, 2009). As students take in information, only so much can be processed through the visual and audio channels. While this is occurring, mental representations are made (Mayer, 2014). Combining multiple representations is confusing for many students (Ainsworth, 2008; Harrison & Treagust, 1996) but unavoidable in chemistry (Nahum et al., 2004). To ease the cognitive load, making connections between representational models (Schnotz, 2005; Seufert, 2003) helps students form these mental models.

### **Chapter Summary**

This literature review began by defining chemical education, discussing what it encompasses as well as the challenges to place the problem statement in the context of the broad field of chemical education. To further introduce the field, a section on chemical educational technology followed by (a) first defining the term, (b) availability and issues, (c) virtual and static models used in chemistry education, and (d) their limitations.

Next, I wanted to support this by discussing chemical education research, leading us to how chemistry is understood. Johnstone's triad is defined next and finished with a discussion on connecting the symbolic and subparticulate levels of chemistry. After introducing elements of chemical education, reaction mechanisms were discussed in terms of importance, issues understanding, and current research around reaction mechanisms. Next, representational model (a) was defined, (b) examples were provided,

and (c) benefits and limitations were discussed. This was followed by an explanation of the types of representational models used in chemistry, including 2D, 3D, concrete, virtual, and using them to connect the symbolic and subparticulate levels of chemistry. Lastly, cognitive learning theory was discussed as the conceptual framework for this study. Here, information processing, schema theory, cognitive load theory, and dual coding were presented.

## CHAPTER 3

### RESEARCH DESIGN

An action research using the convergent mixed methods design was performed to determine if virtual representation supports students understanding and ability to explain a chemical reaction at the symbolic and subparticulate levels (Creswell & Plano Clark, 2017; Mertler, 2020). As an educator, there is a never-ending goal of improving methods to improve student performance and, in this case, improving students' understanding of a chemical reaction and developing a scientific explanation that two of the three models of understanding support. Even when encouraged to do so, students often do not use models to support their explanations (Stull & Hegarty, 2016).

In this mixed methods action study, an insider, such as a teacher or administrator, studied how an aspect of the school functions and implements necessary changes for improvement (Creswell & Creswell, 2018). Action research was an appropriate choice for the purpose of this study as it is not intended to be generalizable but to improve the course. The advantage of action research was the flexibility in the role of the researcher and the control I had as the researcher working in my own space of influence. The researcher gained information on how to readily improve the experience for both the participants and the researcher (Mertler, 2020). This was achieved because action research is a cyclical process wherein the researchers can solve the problem based on the data collected in this study and thereby improve their teaching/learning practices by applying the implications from the study. The iterative nature of the action research was



best for this study because it provided an opportunity to uncover potential errors and change the data collection methods (Fetters, Curry & Creswell, 2013; Sechrest & Sidana, 1995).

This action research study used a convergent mixed method design (Creswell & Plano Clark, 2017). Ultimately, the research questions were a quest in the “pursuit of understanding through recomposition” (Dzurec & Abraham, 1993, p. 76-77). Dzurec and Abraham (1993) identified this as one of six “pursuits” for the use of qualitative and quantitative methods. Combining the two methods confirmed and corroborated data and aided in the development of richer data (Denscombe, 2008; Rossman & Wilson, 1985). Each independent phase of data collection contained concepts that could be compared to another during analysis (Creswell & Plano Clark, 2006; Fetters et al., 2013) to develop the study's findings.

### **Setting and Participants**

This mixed methods action research was conducted at Bellefield High School (BHS), located in a suburban area in the Southeastern United States. BHS was a public high with a population over 1,700 in the 2018-2019 school year. BHS is a one-to-one school using Chromebooks. Chemistry 2 Honors is an elective lab science course that focuses on chemical bonding. Students met every other day across two weeks. The first week students met on Monday, Wednesday, and Friday. The following week students met on Tuesday and Thursday. Students met for a 90-minute session across 36 weeks/two semesters (e.g., Monday, Wednesday, and Friday) for 90-minute sessions across two semesters. The class had a delayed start every Wednesday at the high school, and classes

only met for approximately 70 minutes. A single course section typically consisted of 10 to 25 students.

The normal sequence for the course reviewed Chemical Bonding from Chemistry 1 Honors. Throughout the year, students gained a foundation of carbon compounds and their chemical and physical properties while completing project-based lessons. Laboratories and projects included creating and purifying esters, perfecting the process of saponification for sale, and determining and carrying out procedures for the production and analysis of biodiesel fuel and bioplastics. Students participated in direct instruction, reciprocal instruction, group inquiry activities, laboratory activities, project-based lessons, and independent research in the classroom.

Chemistry 2 Honor students alternated between working in pairs or groups of three for group activities, including in-class projects, lessons, practice, and laboratories. Students indicated their preferences on who they work well with and why by the third week of school. Students were then assigned groups and rarely changed groups throughout the school year by their choice. Materials used throughout the year included periodic tables, concrete molecular modeling kits, access to dynamic 2D virtual molecular models using MolView using a school-issued Chromebook. If a student declined a school-issued device, they were still required to bring their device per our district device policy and to access Google Suites. The assessment for this class included a paper-pencil test (multiple-choice, short response), projects, lab reports, and presentations.

Purposive sampling method was used to recruit the participants for this study. Inclusion criteria for this study included 1) voluntarily consenting to participate in the

study and 2) completing Chemistry 1 Honors with a grade of an A or B or having the recommendation of the Chemistry 1 teacher. The participants for this study included nine students. Students chosen to participate in the study had taken two or three years of chemistry. This year, one student had taken AP Chemistry after Chemistry 1 Honors and were then taking their third year of chemistry in Chemistry 2 Honors. I had taught most of the Chemistry 2 Honors students in Chemistry 1 Honors in the prior two years. Participants' ages ranged from 16 to 18. The break down for ages was 44% of the class was 17 years of age and 56% of the class was 16 years of age. Participants were all Caucasian and 56% of them were female. No students had a 504 accommodation or Individualized Educational Plan. A little less than half of the class were seniors in high school (44%) and the remaining were juniors.

All these participants had been identified as Gifted and Talented. Three participants were not part of the schools' STEM program but were eligible. However, all participants had taken one or more College Board Advanced Placement course in a core content area during their high school career. The class average for Chemistry 1 Honors was 88.9 (B). Seven participants completed Chemistry 1 Honors in the 20-21 school year. The remaining three participants completed Chemistry 1 Honors in the 19-20 school year.

These three participants completed Chemistry 1 Honors virtually as mandated by state Stay at Home orders due to the outbreak of Covid-19. These participants were characterized as high-performing students and had been identified as Gifted and Talented.

### **Innovation**

This section provides details of the innovation used to address the problem of practice. The innovation used in this action research study was the application of virtual

models via MolView.org, a web-based chemical education technology tool that allows students to make virtual models.

### **Overview of the Innovation**

The purpose of using 3D representation was to help students understand the reaction mechanism better by connecting their 2D symbolic drawings to 3D subparticulate virtual models in their articulation of their understanding of the reaction. Students in this Chemistry 2 course have difficulty connecting content represented with symbolic models to the subparticulate level (Czysz et al., 2020; Treagust & Chittleborough, 2001; Treagust et al., 2003). Students may repeat a pattern in a reaction but have difficulty explaining the change at the subparticulate level, including the chemical and physical properties that allow or hinder the reaction (Gilbert & Treagust, 2009). Students tend to explain reactions by identifying patterns within the symbolic models and no connection to the subparticulate level, explaining why the reaction occurs (Bongers et al., 2019, Bhattacharyya, 2014). They often focus on surface features (Bhattacharyya, 2006; Galloway et al., 2017).

Research has shown that the use of animations can help students develop a better understanding of a reaction as it serves as a mental cue (Bongers et al., 2019; Northoff, & Flynn, 2019) and has been shown to change students' mental model of a reaction (Bongers et al., 2020) by moving information from working memory into long-term memory. Animations help students add to their conceptual understanding of traditional 2D Lewis Dot Structures and reaction mechanisms by building from this existing schema to create an intermediate model (Williams & Clement, 2015). To do this, it is important that the virtual models not require extraneous cognitive load to translate between the 2D

models they are familiar with and the new 3D virtual models. Features that the students are not familiar with will distract students (Chen et al., 2017), increasing the extraneous cognitive load which needs to be minimized. Similarities between the new 3D virtual models and familiar 2D models allow students to focus on important subparticulate features and move this information into long-term memory (Kirschner et al., 2018). This transitional conceptual model will help students meet the objective of understanding the target model (Williams & Clement, 2015) and help develop their ability to explain the concept using the 2D static model and the 3D virtual model (Suits & Sanger, 2013; Suits, 2015). As seen in Figure 3.1, using MolView students could manipulate the 3D virtual models by making bond-line-angle drawings and toggling between showing implied atoms or not which are shown in Figure 3.2.

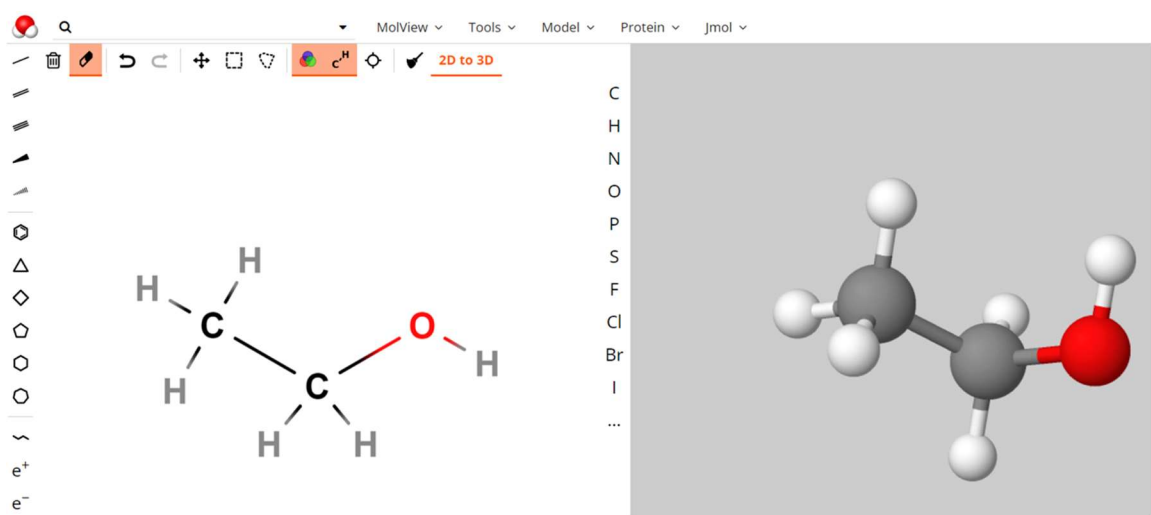


Figure 3.1 2D Virtual (symbolic) Versus Dynamic 3D Virtual (symbolic) Representations

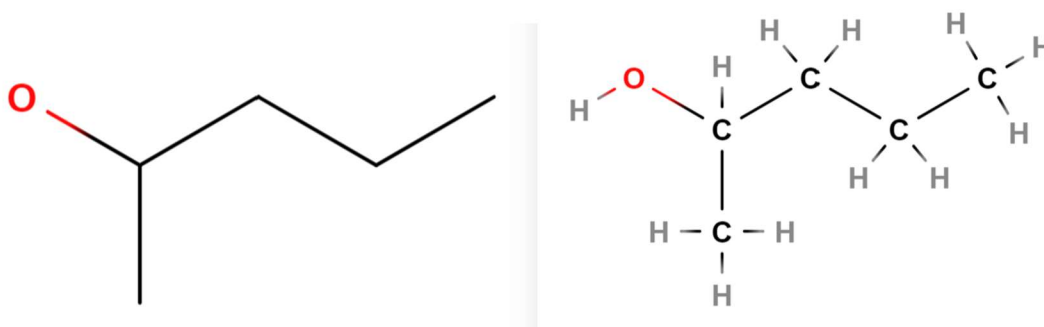


Figure 3.2 Explicit Versus Implied Atoms

*Note.* The left image shows a molecule with implied atoms, hydrogen and carbon not shown. The image on the right shows the same molecular structure with explicit atoms.

In addition to creating 3D virtual models, MolView allowed the students to apply different subparticulate filters to the 3D virtual molecular model. Filters included subparticulate data such as angles, bond dipoles, torsion, charges, and molecular electrostatic potential (MEP or ESP) maps. Figure 3.3 shows the MEP lucent filter (lucent filter).

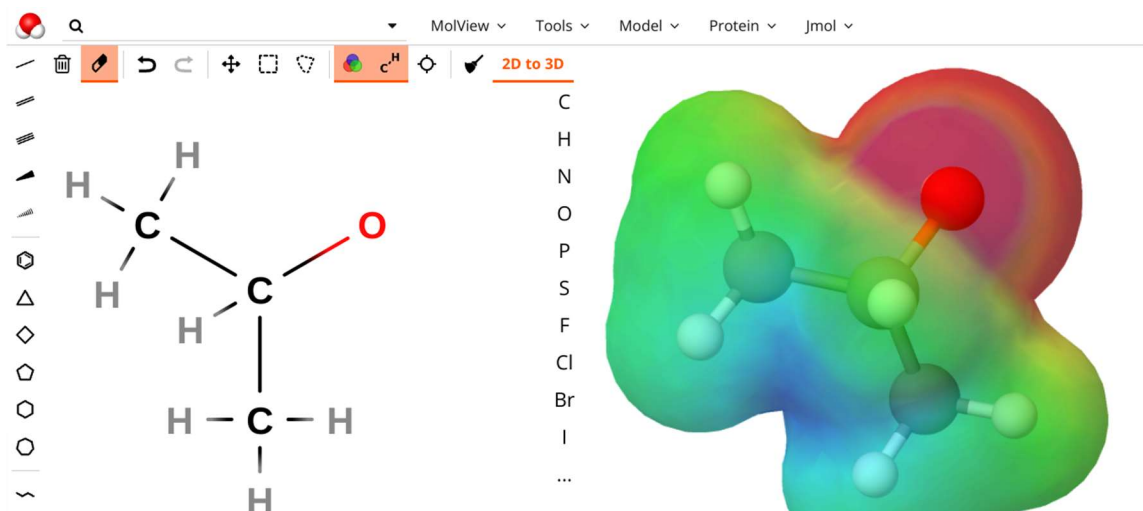


Figure 3.3 Symbolic and Subparticulate Representations of Propanol

The benefit of these filters lied in their visual representation of a concept that, up until this point, had been communicated symbolically through numbers. In addition, this visualization highlights the leap in faith students must make in the subparticulate level to explain observable properties (Al-Balushi & Al-Harthy, 2015; Taber, 2013) and closes

the gap for the student. Following CLT implications, this study implemented practices about different reactants over four to five days with MolView, reinforcing to students understanding of how the reaction occurs by connecting the subparticulate 3D models and the 2D models (Good & Brophy, 1990).

For this innovation, students used MolView to create 3D virtual molecular models that showed subparticulate properties. MolView has a split-screen showing a virtual 2D symbolic model next to a 3D virtual subparticulate model. Having these types of representations on the same screen supported the Dual Coding theory. The side-by-side presentation allowed working memory to develop the translation (understanding) between the two models (Kirschner, 2019). The innovation involved students working in groups of two to aid their conceptual understanding (Rodriguez & Potvin, 2021) of the subparticulate level through discourse (Aldahmash & Abraham, 2009). Working in groups also encouraged discussion and resolution of conflicting perspectives (Howe, 2014). Before students began their group practice, as a whole group, sitting in pairs, there was a review of the 3D virtual model to ensure that students had the time to ask questions about the model before reading it on their own and because explicit instruction of salient and extraneous features helps maximize students' conceptual development (Kelly et al., 2017; Lowe, 2004; Tasker & Dalton, 2008). Part of this was explained in cognitive load theory as the student will not have to spend cognitive load trying to translate between the 2D and 3D or deciphering the 3D model (Brünken et al., 2003; Paas et al., 2003; Clark & Lyons, 2011).

This innovation was implemented in seven sessions across four weeks for a total of seven class meetings. The first day was a pre-innovation introductory session which

took about 10 minutes to introduce students to MolView. The first full day of the innovation entailed a teacher-led activity to activate prior knowledge and how information is presented in MolView. This day also included teacher-modeled use of MolView and guided practice with the reaction mechanism. The teacher modeling of MolView required students to complete very specific tasks. This took a full 90 minutes. After that, we spent six days over seven scheduled classes across three weeks. This fourth day entailed the MolView Group activity which took about 70 minutes. The rest of the innovation took four more days. The bellwork practice on the first day took about 25 minutes including review time. At the end of the seventh day of the innovation and the bellwork practice took about seven to ten minutes with little review.

### **Description of the Innovation**

The innovation was composed of several events, including the objectives, prior knowledge, MolView instructor modeling, guided practice, a MolView small group activity and several days of continued practice using MolView. This next section describes each event in sequence.

#### ***MolView Orientation***

This section describes components of the orientation phase. During this time, the use of MolView corresponded to dual coding theory. Later in this phase, schema theory and cognitive load theory were applied as students learned to connect abstract chemical concepts in 3D subparticulate representations to 2D symbolic drawings they had worked with for the last year.

**Objectives.** Students were arranged in pairs on the first day of implementing 3D dynamic molecular modeling using MolView. MolView was selected because its split



screen makes use of dual coding theory and minimizes the capacity required for working memory (Clark & Lyons, 2011). Seats were moved next to each other, separate from other pairs. Desks were facing the Smartboard providing the start of day instructions for seating arrangement and the title of the day's assignment MolView Introduction Activity in Google Classroom. Students logged into Google Classroom to access the assignment and assignment document with their partner. Students picked their partner for the day's lesson. Students first reviewed the instructions for the assignment after the same document was presented on the Smartboard to the entire class. The objectives for the intervention were then reviewed. These included

- 1) I can read an 3D virtual molecular model to indicate areas of high and low electron density,
- 2) I can identify an area on one molecule that would be electrostatically attracted to another area of a different molecule,
- 3) I can explain the areas of high and low electron density due to bond polarity and electronegativity differences or formal charges.

Students were then instructed on where and how to submit the day's work. This took approximately five minutes.

**Prior Knowledge.** Students were then be presented with a temperature map of the world from Global Temperatures from Weather Underground (2022). Students were asked to first think about the following questions:

- What is this map about?
- What information does it provide?
- How do you know?

The map was reviewed as a whole group. Emphasis was placed on modeling information by using color coding and using students' prior knowledge (the poles are cold; the equator is warm) to explain models. This step was important because there was about to be a large amount of new information presented. To minimize cognitive load and maximize working memory, the new information had to be tied to old schemata and included familiar imagery (Jung et al., 2022; Kirschner et al., 2018; Neumann & Kopcha, 2018 Sweller et al., 2011).

### ***MolView Instructor Modeling***

Next, MolView was displayed on the Smartboard, and students were asked to draw the structure for methanol on MolView. They all had the option of creating a 2D structural model on paper first, as they have done throughout the year, then in MolView. After checking the students' structures in MolView, methanol was created using MolView on the Smartboard for all students to see. After showing students how to use MolView's "clean up" feature, they were then showed how to convert the 2D virtual MolView structure to a 3D virtual structure that can be manipulated by the student using a touch screen or touch pad. Using methanol, how to 1) manipulate the 3D molecular structure and 2) convert the 3D molecular structure into an electrostatic molecular structure was modeled for students on the SmartBoard. The students did the same on their screens, using their Chromebook afterwards. Students are then instructed to click the clean-up icon, 2D-3D icon, then open the Jmol dropdown menu at the top of the page. From the dropdown menu, they selected "MEP surface lucent" or lucent filter (as seen in Figure 3.4 above). From this 3D virtual model, students were instructed to rotate the molecule and note the heat map coloring of the applied lucent filter. The use of the lucent

filter activated schema related to heat maps. This created the opportunity to connect the lucent filter to electronegativity and formal charges by making use of CLT. The lucent filter helped move the abstract concepts of formal charges and electronegativity into long-term memory by providing a visual aid that did not increase the intrinsic cognitive load of the participants nor increase extrinsic cognitive load. At this time, it was determined that students had applied the correct filter to the 3D molecular structure and could manipulate the structure using the mouse pad of the Chromebook by visual inspection and chit chat.

The next step in the activity was for students to evaluate the meaning of the colors of the electrostatic potential map or lucent filter- “How would you explain the different colors of the 3D structure?” As needed, the prompts below were asked.

T: Is there a difference between the atoms in red and those in blue?

St: yes/no

T: In what ways are those atoms different at the subparticulate level?

St: size/ formal charge/ electronegativity/ position

T: What does a heat map indicate?

St: hot and cold, difference in temperature

T: If hot and cold are opposites, what properties could two atoms or sides of a molecule have that could be considered opposites?

This took 30 minutes with a small-sized class of nine students.

### ***Guided Practice***

Once all students were able to indicate the relationship between the color and electronegativity or formal charge, evaluated by directly asking the students and listening

to their discussions with partners and other class members, they were asked if the colors reflect changes in electron density to guide the achievement of “I Can” statements One and Three. To further ensure all students had attained this goal, each group was assigned a small molecule to draw in MolView and convert its 3D model to the lucent filter model. Molecules included water, fluoroethane, propanone, benzene, and hept-2-yne. These molecules were selected because they met at least one criterion that highlighted electrostatic potential differences with the lucent filter on display: molecular polarity, bond polarity and pi electrons. Students were then asked to discuss the subparticulate level properties indicated in the 3D molecular model (right side of the screen). They did this with their group first then shared their thought process with the rest of the class as part of a whole group discussion initiated by asking the whole group and waiting for responses. The purpose here was to allow students to witness and discuss the ESP maps (3D models with the lucent filter) of different molecules and determine that electron density drives the coloring of the 3D ESP models. Once most students were able to describe the 3D subparticulate model in terms of electronegativity or pi-bonding (determined by small and whole-group discussion) using an informal check on their perception of their understanding using a thumb up, sideways, or down indication. The time frame for this component of the innovation was 30 minutes.

At this time, still in partners, the reaction mechanism for the Fischer Esterification of ethanol (an alcohol) and ethanoic acid (a carboxylic acid) using an acid catalyst was introduced as whole group instruction. Students were guided through this reaction mechanism by toggling between the document camera and MolView. For each step, the 2D symbolic representation of the reacting molecules was drawn first. Formal charges

were calculated for intermediates by hand on the symbolic structures displayed by the document camera. The molecules were built in MolView and displayed on the SmartBoard for each step of the reaction mechanism. Students were then asked to discuss then respond to the question “Where could these molecules be attracted to each other?” as in Figure 3.4 below.

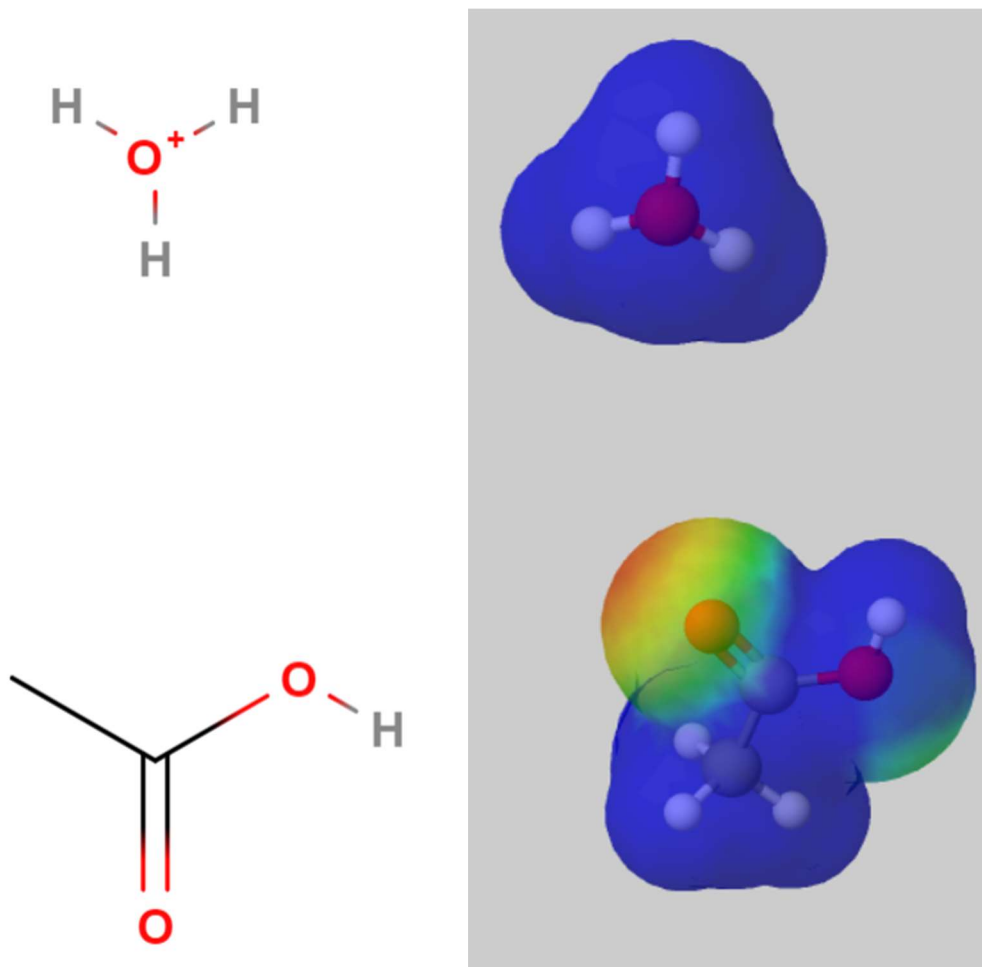


Figure 3.4 Starting Materials for Acid Catalyzed Fischer Esterification  
Note: The left models the 2D virtual model (symbolic) and the right models the subparticulate representation of each molecule's electron density. Red indicates high electron density and blue low density.

Over the duration of this guided practice and one more example reaction, students viewed a molecule in MolView and saw the 3D lucent filter to identify high and low

areas of electron density to predict where molecules could react with each other. Using this line of questioning, students were introduced to electron pushing formalism, a notation using curved arrows indicating the flow or movement of electrons from high to low electron dense regions between molecules (Bongers et al., 2019). This is the notation used in reaction mechanisms and considered one of the most important tools in organic chemistry (Bodner, 2015).

### ***MolView Small Group Activity***

For the second “I Can” statement, students were asked to recall the importance of resonance structures from prior units. Resonance structures are important because they provide a chemist insight as to what part(s) of a molecule may be reactive (Klein, 2022). Students, while working with their class partner, created the 3D molecular structures for methanol and propanoic acid. At this time, students began recording their screen and sound using Screencastify. They discussed what they were seeing in MolView and were prompted with questions such as “Is it possible to predict if two molecules could react or not and where the reaction sites would be?” Students took screenshots of these images, using the Chromebook’s screenshot tool and added them to their assignment in Google Classroom- MolView Group Activity. They drew arrows between molecules to indicate where one would react with the other, as done in electron pushing formalism. At this time, the direction of the arrow was not emphasized or corrected because the primary objective was for students to learn to read the 3D lucent filter and apply that information to their symbolic structures. The Screencastify video was submitted in the same Google Classroom assignment. The instructor's role was to facilitate their progress with questions. This activity took 35-45 minutes.

## ***Practice***

Once students had completed the MolView small group activity, they began their reading assignment on the types of compounds they have been working with during the activity. Content related to the compounds of the reaction were covered over the next seven days after Google Classroom posted bellwork assignments on reaction mechanisms using MolView. This followed the routine of independent reading, direct instruction and independent/small group practice of the reactants and products' properties and uses (see Table 3.1).

**Table 3.1 Topics and Practice Covered After MolView Introduction**

Stage	Description
Day 1 Pre-Innovation	Whole Group: Study is explained Whole Group: Orientation of MolView
Day 2 Pre-Innovation	Individual: Entry point knowledge & Pre-assessment Collection of demographics Whole Group: Introducing the scope and purpose of the unit
Day 3 Innovation Introduction	Whole group: Activating prior knowledge Whole group direct instruction: MolView instructor modeling Whole group: Guided practice of reaction mechanism with intermediates in MolView
Day 4 Innovation	Whole group student led: Review of guided reaction mechanism practice with intermediates in MolView Small group: MolView small group activity
Day 5 Innovation Practice & Content	Small/whole group bellwork practice: 2 ester reactions with MolView Independent/small group practice: Readings on alcohols, phenol, naming phenols Independent/small group work: Properties of alcohols, phenols, naming, practice esterification reaction mechanism with MolView

---

Day 6 Innovation Practice & Content	<p>Small/whole group bellwork practice: Practice esterification reaction mechanism with MolView</p> <p>Whole group student led: Review esterification reactions</p> <p>Whole group direct instruction: Substitution of alcohols</p> <p>Reactions: dehydration of an alcohol, ether formation, oxidation of an alcohol (primary, secondary)</p> <p>Independent/small group practice: New reactions</p>
Day 7 Innovation Practice & Content	<p>Small/whole group bellwork practice: Practice esterification reaction mechanism with MolView</p> <p>Whole group: Review esterification reactions</p> <p>Independent/small group practice: Reading-carboxylic acids-properties, solubility, organic acid intro, neutralization. Esters- properties, naming, solubility, base hydrolysis of esters (saponification),</p>
Day 8 Innovation Practice & Content	<p>Small/whole group bellwork practice: Practice esterification reaction mechanism with MolView</p> <p>Whole group: Review esterification reactions</p> <p>Independent/small group practice: carboxylic acids-properties, solubility, organic acid intro, neutralization. Esters- properties, naming, solubility, base hydrolysis of esters (saponification)</p>
Day 9 Assessment	Independent: Short response assessment
Day 10 Content Review	<p>Small group teacher led: Review of short response assessment</p> <p>Independent/small group: Begin esterification procedures online search</p>
Day 11 Post-Unit	Independent: Post-assessment
Day 12-20 Post-Unit	<p>Individual interviews</p> <p>Articulation assessment</p>
Data Analysis	<p>Descriptive statistics</p> <p>Wilcoxon Signed Rank test</p> <p>Inductive analysis</p>

---



Reporting	Participants Administrators Chemistry and Physical Science teachers
-----------	---

During this time, students had the opportunity to continue working with MolView to practice predicting products and the reaction mechanism. Once students had time to cover and practice the remaining unit content listed in days five through nine of Table 3.1, participants took the post assessment.

### Data Collection

To answer the research questions, the unit consisted of multiple data sources of how students explored molecules and electrons at various levels of modeling, as demonstrated in Figure 3.5. Table 3.2 shows the research question alignment with data collection methods.

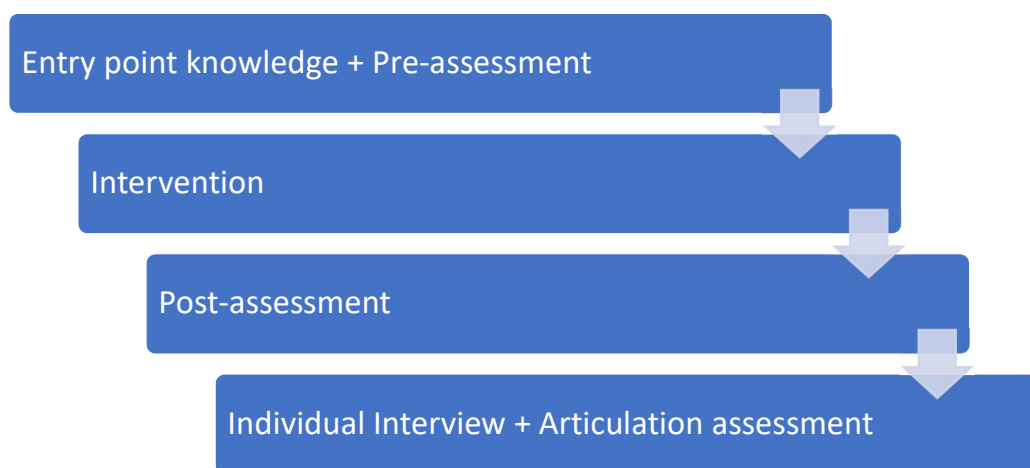


Figure 3.5 Sequencing of Events for the Study

Table 3.2 Research Question and Data Source Alignment Table

Research Questions	Data Source
How does students' ability to complete a reaction mechanism change after using 3D models to explore the symbolic and subparticulate representational levels of chemistry?	Pre- post-assessment test Individual interview Articulation assessment

How do students articulate the process of a reaction mechanism after manipulating 3D virtual models?	Individual interview Articulation assessment
What is the students' perception of using 3D models to learn a chemical reaction?	Individual interview

This section will review the types of data collection methods used in this mixed methods study. This section first discusses quantitative methods followed by qualitative sources.

## **Quantitative Data**

### ***Entry Point Knowledge Check***

An entry point knowledge check (see Appendix A) was used to confirm participant understanding of required prior knowledge. The entry point knowledge check provided information on instructional content that may need to be reviewed before formally beginning the unit and innovation. The scoring for this test did not count towards the student's grade in the course. The entry point knowledge check was completed after the instructor's explanation of the study. Students submitted their responses on the printed assessment. Ten participants completed this assessment at the beginning of this innovation unit, but only responses from the nine participants who completed the study were included for data analysis.

The entry point knowledge check was a teacher-developed assessment and based on the objectives in Table 3.3. The test will include 12 questions in total. Six questions were multiple choice and five were short response. Each multiple-choice was worth one point, question 12 was split into 12a and 12b. The point value for the short response range from zero to one point. Six of the short response questions are worth one point because there was only one correct response. The entry point knowledge check was worth

a total of 13 points. These questions establish content knowledge base on electronegativity, formal charge (FC), calculation, functional groups, types of compounds, and electron density. A rubric for this section follows.

Table 3.3 Entry Point Knowledge Assessment and Objectives Table

Objective	Content Knowledge	Number of Items	Item Number
1. Students will be able to compare relative electronegativities of sets of atoms	Identify the high or low electronegativity from a pair of atoms- nonmetals	2	1,2
2. Students will be able to distinguish between three functional groups.	Identifying functional groups (carboxyl, carbonyl, hydroxyl)	3	3-5
3. Students will be able to distinguish between three classes of compounds	Identify classes of compounds (alcohol, ester, carboxylic acid)	4	6-9
4. Students will be able to calculate the FC of an indicated atom	Calculate formal charge	2	10, 11
5. Students will be able to predict areas of high and low electron density	Identify areas of high and low electron density	1	12
12		Total	

The internal consistency reliability of the test items was determined using *Kuder-Richardson 20 (KR-20)*.

### ***Pre Post-Assessment***

The four open-ended reaction mechanism questions completed by the nine participants are presented next. The four open-ended Fischer Esterification reaction mechanisms accompanied the entry point knowledge check. The cumulative unit assessment, given at the end of the unit, repeated the four open-ended Fischer

Esterification reaction mechanisms alongside other content-related questions, such as properties of the compounds and uses. Objectives and content knowledge are aligned in Table 3.4 below.

Table 3.4 Pre-post assessment and Objectives Table

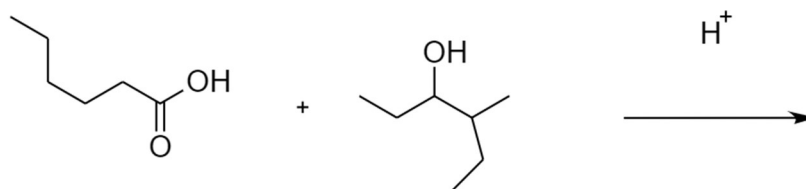
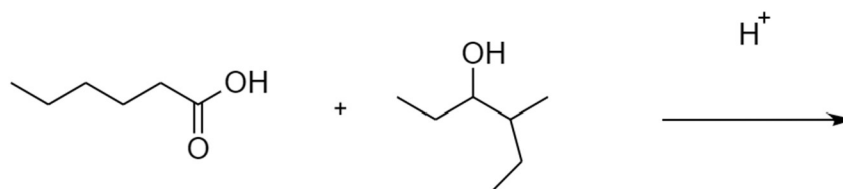
Objective	Content Knowledge	Number of Items
Students will be able to predict the products of an esterification reaction	Predict the reaction mechanism for the product of an ester	4

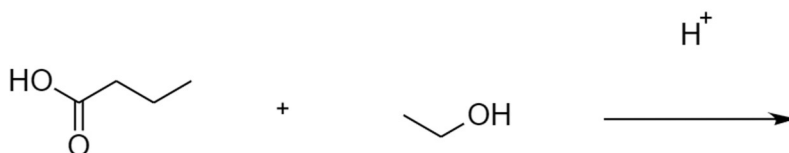
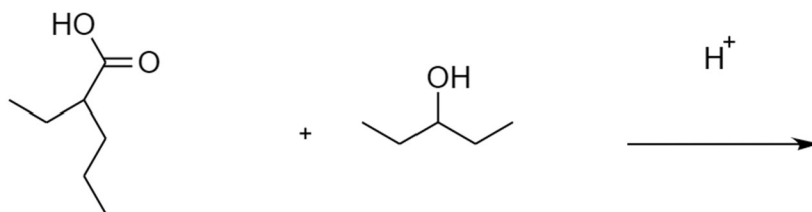
The unit assessment was administered after students had worked with the 3D virtual representation for seven class meetings or three weeks.

The remaining four questions (see Table 3.5) cover reaction mechanisms and were assessed on product formation, electron pushing formalism, formal charges, and intermediates.

Table 3.5 Reactants for the Pre-post assessment

Instructions: Draw the mechanism and product(s) of this reaction






---

Each criterion was scored on a one to five-point scale. One point was assigned if the question was not attempted. A maximum of five points were assigned for the correct product, electron pushing formalism, formal charges, and intermediates each. A total of 80 points were possible.

One chemistry teacher at my school validated the questions, the rubric, and the grading procedures. In addition, inter-rater reliability of the open-ended pre- and post-assessment questions was assessed by the Cohen's (1960) kappa coefficient. The pre-post assessment items are available in Appendix A, items #13-16.

### ***Student Articulation***

This study quantified data from qualitative measures of students' articulation on students' ability to explain the reaction and concepts around the reaction using appropriate theory and logic. Quantization was used to communicate accuracy and find patterns in their understanding of the content (Sandelowski et al., 2009). During the assessment, the assessor can collect more in-depth responses (Johnson, 2002) and

quantize this complicated information then increased objectivity in students' ability to present their understanding of the concepts (Chi, 1997). Students had the opportunity to think through their process aloud and describe how they understood the concepts and developed their answers to the open-ended post-assessment questions.

This study asked students to explain how they determined the product of a chemical reaction and their understanding of electron pushing formalism and formal charges as part of the interview at the end of the unit. These interview questions were asked about the open-ended reaction mechanisms that were part of the cumulative unit assessment, while their work was in front of them during the recording. If students had memorized a pattern, they would not address subparticulate properties visible in the 3D virtual molecular models. Their responses revealed what levels of understanding were used most or not at all.

To ensure the information needed was gathered with the necessary detail, prompts were included (Creswell & Creswell, 2018). The content interview questions (not the reaction) and prompts were pulled from Bongers et al. (2019) to establish validity. The question and prompts are presented in Table 3.6 aligned with the research question. Together, the scripted questions and prompts to make the student's depth of understanding visible.

Table 3.6 Articulation Assessments Question and Prompt Alignment to Research Questions

Articulation Questions and Prompts	Research Question
How did you approach this question? <sup>a</sup>	RQ2: How do students articulate the process of a reaction mechanism after manipulating 3D virtual models?
Can you tell me about the mechanistic arrows that you drew? <sup>a</sup>	
Why do you think the reaction happens at this oxygen (oxygen from the alcohol)	

---

and this carbon (carbon 1 of the carboxylic acid)<sup>b</sup>?

Does the FC of the atom change?

What are the functional groups in the molecule?

Can you tell me more about your transition state structure?<sup>a</sup>

What do you think “transition state structure” means?<sup>a</sup>

---

<sup>a</sup>Interview prompts and question from Bongers et al. (2019)

<sup>b</sup>Modified question from Bongers et al. (2019) to fit the reaction of this study

## Qualitative Data

### *Interview*

All participants were asked to participate in a semi-structured interview once the lesson was completed. The goal was to gather information about the students’ learning experience through the unit. The question and prompts are presented in Table 3.7 and aligned with the research question.

Table 3.7 Alignment of Interview Questions and Research Question

Research Question	Interview Question & Prompt
RQ3 What is the students’ perception of using 3D models to learn a chemical reaction	How did you feel about the entire unit, the content, MolView and your performance?  Did you find MolView to be difficult at any point? Why or why not? Which type of model did you find more useful, 2D drawn models or 3D virtual models? Are there challenges with either and if so, what are they? Explain. Do you have a preference? Could the 3D representation be useful to you in the future? (for other chemistry courses)

RQ1 How does students' ability to complete a reaction mechanism change after using 3D models to explore the symbolic and subparticulate representational levels of chemistry?

How did the 3D representation help you develop your understanding of formal charges and electronegativity? Did it make it more difficult to understand?

Did you understand the reaction differently after the 3D representation? Please explain why.

Do you think you understand why the reaction occurs at the sites it does? Please explain why.

How did you feel you performed on the written test compared to how you actually performed? Explain any discrepancies between the two if any.

Do you think the 3D representation hindered your performance? Please explain why.

If you performed as you expected, did the 3D representation activities help with your performance? Please explain why.

RQ2: How do students articulate the process of a reaction mechanism after manipulating 3D virtual models?

How did you feel you performed on the short response oral assessment compared to how you actually performed? Explain any discrepancies between the two if any.

Do you think the 3D representation hindered your performance? Please explain why.

If you performed as you expected, did the 3D representation activities help with your performance? Please explain why.

---

Criteria for selection required that students attend and complete all activities for the study. While nine participants met these criteria, due to time, only six were purposively selected to participate in the interview. Interviews were held during the regular class meeting times and students volunteered to start interviews each day. The interview occurred after the cumulative unit test with post-assessment questions had been administered and students had received scores for this assessment. This data source



aimed to collect information on the perceived effectiveness of the 3D molecular models (Adeoye-Olatunde & Olenik, 2021). It was an appropriate collection method as the intent of action research was not for generalization (Mertler, 2020), and the student's perspective will provide valuable insight (Adeoye-Olatunde & Olenik, 2021). A semi-structured format was used to allow follow-up questions depending on how students respond (Mertler, 2020). This less structured approach helped students feel more comfortable by being more like a conversation than an assessment (Hamilton & Finley, 2019). This helped create a more accurate description of their experience, ability to articulate their understanding of the concepts and create a rich, thick description of the qualitative analysis. Each session lasted approximately 10-20 minutes and was recorded using a laptop computer for audio and video upon the participant's approval. Transcripts were made using these recordings.

### **Data Analysis**

In this mixed methods action research study, I used descriptive statistics and inferential statistics to analyze quantitative data (e.g., an entry point knowledge check, pre-post assessment, and articulation assessment) (see Table 3.8). For qualitative data, inductive analysis was used to make sense of the participants' responses.

Table 3.8 Research Question and Data Source Alignment Table

Research Question	Data Source	Data Analysis
RQ1 How does students' ability to complete a reaction mechanism change after using 3D models to explore the symbolic and subparticulate representational levels of chemistry?	Pre-post assessment	Descriptive statistics Wilcoxon signed rank test
	Student articulation	Descriptive statistics
	Interview	Inductive analysis

RQ2 How do students articulate the process of a reaction mechanism after manipulating 3D virtual models?	Student articulation	Descriptive statistics
	Interview	Inductive analysis
RQ3 What is the students' perception of using 3D models to learn a chemical reaction?	Interview	Inductive analysis

## Quantitative Data Analysis

### *Entry Point Knowledge Checks*

The multiple-choice instrument completed by all participating students was used to assess students' content knowledge. Internal consistency reliability was checked using Kuder-Richardson 20. Descriptive statistics was provided to assure participants' level of prior knowledge met the requirement for this intervention.

### *Pre-Post Assessment*

Descriptive statistics were used to present the central tendency of the participants' scores in pre-post assessment. Cohen's Kappa was used for interrater reliability, then the Wilcoxon signed rank test with a significance level of  $\alpha = 0.05$  was used to determine if knowledge gains are statistically significant when comparing pre-test and post-test data.

The grading scale for the pre-post assessment of the open-ended reaction mechanism questions is as follows in Table 3.9.

Table 3.9 Rubric for Pre-Post Assessment of Open-Ended Reaction Mechanism Questions

Criterion	1	2	3	4	5
Product	No attempt	Ester is formed but incorrect		Minor error (missing or misplaced substituent)	Correct
electron pushing formalism	No attempt	Three are missing or incorrect	Two are missing or incorrect	One arrow is missing/added	Correct

Formal charge	No attempt	Three are missing or incorrect	Two are missing or incorrect	One FC is missing or added	Correct
Intermediate	No attempt	Three are missing or incorrect	Two are missing or incorrect	One intermediate is incorrect/missing	Correct

### ***Student Articulation***

Qualitative data can be represented in quantitative terms as a means of collecting data in context or data that is more complex (Chi, 1997). For the articulation assessment, a rubric was developed reflecting the components indicated by College Board (2011), Next Generation Science Standards (NGSS) and the National Research Council (NRC) as described in Seeratan et al. (2020) and was adapted from Yao and Guo (2018) to address the theory behind reaction mechanisms. This allowed the qualitative data to be converted into quantitative data for analysis. Table 3.10 presents the alignment between practices used by NGSS, College Board and Yao and Guo's (2018) rubric. Two components from Yao and Guo (2018) were based on NGSS/NRC (Council, 2012) practice frameworks for articulating understanding and making sense of phenomena as described in Seeratan et al. (2020).

Table 3.10 Rubric Alignment with NGSS and College Board

Yao & Guo (2018)	NGSS/NRC Practice (Council, 2012)	Target AP Science Practice (College Board, 2011a)
Full Explanation [of concept]	Component: Articulating understanding	
	Practice: Constructing explanation	Practice: The student can construct explanations of phenomena based on evidence [in this case theory]

Phenomenon Theory [explains concepts]	Component: Make sense of phenomenon	
	Practice: Analyzing and interpreting data [data here are the reactants; interpreting is of the reaction mechanism]	Practice: The student can analyze data to identify patterns or relationships

Articulation assessed students Full Explanation (Explanation) of their understanding of the concept, the reaction mechanism. To explain the reaction mechanism, students needed to explain the Phenomena Theories (Theories) behind the concept of predicting a reaction mechanism including the reaction itself, its' the intermediates, electron pushing formalism, and electron density. Using the criterion in the above Table 3.11, students' ability to articulate their understanding of the following three concepts using appropriate theory as described in Table 3.12 were assessed. Table 3.11 presents Yao and Guo (2018) articulation assessment followed by a more detailed explanation of what this study looked for to assess articulation (Table 3.12, below), including question prompts to elicit students understanding.

Table 3.11 Rubric for Content Related Interview Questions

Yao & Guo (2018)		Description
Full Explanation [of concept]		
2	Students develop an appropriate scientific explanation [the explanation is based on correct and sufficient theory and data, and has logically sound reasoning]	
1	Student constructs an explanation from a scientific perspective, but the explanation is not complete or appropriate	
0	Student gives a wrong explanation	
Phenomenon Theory [explains concepts]		
2	Students explanation is based on theories.	
1	Students explanation is based on insufficient theory (only based on one of the above theories)	

- 0 Students explanation exhibits misunderstanding of the above theories:  
students' explanation is based on inappropriate theory

This data collection method evaluated if students articulated understanding of the concepts by using correct and sufficient theory to make sense of the concepts. They were assessed by listening to their explanations of the reaction mechanism (item #1), electron pushing formalism (EPF, item #2) and formal charges (item #3). For example, I listened for students to connect their explanation of electron pushing formalism and connecting it to high and low electron densities.

Table 3.12 Concept Descriptions and Objectives for Student Articulation

Concepts	Concept Interview Question and Prompts	Accepted Theories	Objective
Reaction mechanism	<p>How did you approach this question? <sup>a</sup></p> <p>Can you tell me about the mechanistic arrows that you drew?<sup>a</sup></p> <p>Why do you think the reaction happens at this oxygen (oxygen from the alcohol) and this carbon (carbon 1 of the carboxylic acid)<sup>b</sup>?</p> <p>Can you tell me more about your transition state structure?<sup>a</sup></p> <p>What do you think “transition state structure” means? <sup>a</sup></p>	<p>Explanation of thought process in working through the reaction mechanism or portion of reaction mechanism</p>	<p>Students can accurately discuss formal charges, electron pushing formalism, or resonance as theories behind the reaction mechanism</p>
Electron pushing formalism	<p>Can you tell me about the mechanistic arrows that you drew?<sup>a</sup></p>	<p>Explanation of electron pushing formalism used in</p>	<p>Students can accurately discuss electron pushing</p>

	<p>Why do you think the reaction happens at this oxygen (oxygen from the alcohol) and this carbon (carbon 1 of the carboxylic acid)<sup>b</sup>?</p> <p>Can you tell me more about your transition state structure?<sup>a</sup></p> <p>What do you think “transition state structure” means?<sup>a</sup></p>	<p>the reaction mechanism</p>	<p>formalism and the “movement” of electrons from high to low electron dense regions to create more stable structures as theories behind the reaction mechanism</p>
Formal Charges	<p>Why do you think the reaction happens at this oxygen (oxygen from the alcohol) and this carbon (carbon 1 of the carboxylic acid)<sup>b</sup>?</p> <p>Does the FC of the atom change?</p>	<p>Explanation of impact of formal charges on predicting or working through reaction mechanism</p>	<p>Students can accurately discuss FC and electronegativity as indicators of high and low electron dense regions as theories behind the reaction mechanism</p>

---

### Qualitative Data Analysis

This study used an inductive analysis of the qualitative data collected from the interview. Process coding and in vivo coding were used for RQ3 to actively answer this question. After transcribing the interviews from Happy Scribe and into Delve, first cycle coding began. These codes were the foundation of the coding scheme in the second cycle. The coding scheme allowed similar items to be grouped together (Parsons & Brown, 2002; Saldaña, 2009) to identify themes. While there was an end goal, the coding process was cyclical and required more than three rounds per cycle (Saldaña, 2009) of revisions

to reassess pattern codes, categories, and themes. The focus remained on developing patterns of the students' experience using the 3D representation, using other models, and how they understood the concepts of the reaction mechanism.

### Procedures and Timeline

The following section begins with a table outlining the timeline and what occurred for each phase in Table 3.13. Each step is then described, including the (a) pre-innovation, (b) innovation, (c) practice, (d) assessment, (e) post-unit, (f) data analysis and finally, (g) reporting.

Table 3.13 Stage Description and Timetable

Stage	Description
Pre-Innovation (two class session)	Study was explained as a whole group Orientation to MolView Entry point knowledge check with pre-assessment questions Collection of demographics Introducing the scope and purpose of the unit
Innovation Introduction (one class session)	As a whole group, prior knowledge was activated followed by teacher guided practice using MolView and reaction mechanisms and intermediates.
Innovation (one class session)	As a whole group, students led a review of the reaction mechanism with intermediates in MolView  In small groups, students began MolView Small Group Activity
Innovation Practice & Content (four class sessions/ two weeks)	Bellwork practicing two reaction mechanisms in MolView Independent/small group practice on alcohols, phenols, esters, carboxylic acids, naming, properties, substitution of alcohols, organic acid intro, neutralization reactions
Assessment & Reviews (three class sessions)	Short response assessment of esterification reaction mechanisms with individual feedback & whole group review Unit assessment with post-assessment questions

Post-Unit (nine class sessions/ four weeks)	Individual interviews
Data Analysis	Descriptive statistics Wilcoxon signed rank test Inductive analysis
Reporting	Participants Administrators Chemistry and Physical Science teachers

---

For the study, all students were invited to participate. While ten students were enrolled, nine participated in the content knowledge assessment, pre-post assessment, and MolView Small Group Activity. Of those students, six were interviewed to collect qualitative and quantitative interview data. There was one student that was present for the study orientation but was no longer in attendance for all other components of the study. Only six of the nine participants were interviewed because as the time between the unit and the interviews increased, memories of what was helpful began to fail. For this study, my part as the researcher would be considered full participation. It proved to be the most natural option as I was the classroom teacher and had a working history with many participants. This approach also helped support the credibility of this research (Mertler, 2020).

### **Pre-innovation**

This phase introduced the study to students. Students were not required to participate but did receive the same assessments and innovation regardless. Once the purpose of the study and the scope of the unit were explained, students had an opportunity to ask questions. This was followed by the paper-pencil entry point knowledge check with pre-assessment questions. The introduction to the study occurred during the last 60 minutes of a class session.



## **Innovation**

During this stage of the study, students started with a question to prompt prior knowledge of symbolic representations of a global heat map. Objectives for the unit and “I can” statements for the activity were reviewed. Next, as students sat with their partner, they followed along with instructor-modeling of how to convert 2D virtual structures to 3D virtual structures that can be manipulated. Together, each group created a molecule in MolView. Students were then prompted to discuss why the structures had the ESP maps. Once students had created and manipulated a 3D virtual model on their Chromebook in pairs, they completed an activity to be submitted electronically.

## **Practice**

After the innovation had been introduced, students were engaged in direct instruction and individual and small group practice with the reaction and 3D modeling. Practice was reviewed before students left for the day or reviewed as a whole group. This formative practice was not graded but served to provide feedback. This portion took four class meetings or two weeks.

## **Assessment**

The assessment component was composed of three collection methods that began once the content had been delivered and students had time to practice. This next section details the post-assessment, interview, and articulation assessment.

The post-assessment occurred after the innovation had been introduced, students had practiced, and the remainder of the content had been covered. It took place in the regular classroom. Students were in their assigned seats which were lined up in rows. The post-assessment will be part of a more extensive end of unit multiple-choice, short-

response test covering other components of the unit and the reaction. Students had a total of 90 minutes to complete the assessment. Answers were recorded on paper.

The interviews took place in the hallway. Interviews began the day after the post-assessment. The format and materials for the interview were first explained in the classroom, taking approximately ten minutes. The interviews were administered one at a time. Students that were not testing remained in the classroom. The door was left ajar, and students were seated facing away from the door to minimize distractions. This also allowed me to see into the classroom. Once students had the opportunity to ask any questions pertaining to the format of the assessment, the assessment began.

At the start of the interview, once outside of the classroom, the computer recording of the assessment was started using Screencastify. Students received a hard copy of their original work. The interview began with questions to ease into the conversation and a reminder that their perspective did not affect their grade in the course. Once students completed the interview, they returned to the classroom and the next student entered the hallway to me with me. Once the recordings were completed, they were transcribed and reviewed for accuracy.

Articulation was assessed after the post-assessment. Students verbally explained their process for completing a reaction mechanism, electron pushing formalism, and formal charges. Data collection followed the same procedures as the interview, outside of the classroom and with a copy of their work on the recording device and the original hard copy in front of them to review. The recordings were transcribed once students completed the assessment. These were checked for accuracy of explanation, usage of electron pushing formalism, (EPF), calculation of formal charges, and intermediate products to

contribute to the quantitative data. Each interview took about 10 to 18 minutes. It was completed over four weeks or ten class sessions.

### **Post Unit**

The post unit included interviews and articulation assessments with six students. At this time, students had received feedback on their assessments. Students were asked questions such as (a) how they felt using the 3D virtual MolView modeling, (b) if they felt it helped them understand the reaction, (c) if it was reflected in their assessments, and (d) about their thought process for portions of a reaction mechanism. A complete list of questions for the articulation assessment are in Table 3.6 and interview questions in Table 3.7. This data was compared to the quantitative data for integration and to create the thick, rich descriptive narrative.

### **Data Analysis**

This stage of the study included data analysis of the quantitative and qualitative methods using inductive analysis, Wilcoxon signed rank test, descriptive statistics. At this time, all components requiring student input had been concluded.

### **Reporting of Results**

Once data analysis has concluded, the results were shared first with the students that were still at the school, as they were juniors and had not moved away. This was done during the school day that most of us were able to meet. The next opportunity to report the results of the mixed methods action study was with the assistant principal of instruction and the school digital integration specialist (DIS). This meeting was set up during school hours during a common planning time. The last meeting was with chemistry teachers within the department. Discussions included the benefits or lack of

benefits to student performance, recommended modifications to instruction or opportunities for further study.

### **Rigor & Trustworthiness**

For the data in this mixed methods study, several methods were used to ensure rigor and trustworthiness. By using a variety of data sources, thick, rich descriptions, and utilizing both member checking and peer debriefing, this “help[ed] ensure the trustworthiness of [my] data” (Mertler, 2020, p. 142).

### **Triangulation**

Triangulation uses multiple data sources and methods to help decrease or eliminate bias and increase the validity of the study (Jonsen & Jehn, 2009). This was done by comparing my quantitative pre-post assessment and articulation data to the information gathered from the interviews. This allowed me to ensure that the variance in the data collected was due to the traits rather than the research method (Jick, 1979). Triangulation also explained why the participants answered the interview questions as they did. This allows for another layer of clarification to ensure accuracy and credibility (Mertler, 2020).

### **Member Checking**

Member checking was used to increase rigor and trustworthiness by having some participants review the findings from the post-assessment and interview (Creswell, 2014; Creswell & Creswell, 2018; Tracy, 2020). This helped verify that my interpretations of the data gathered accurately represent participants’ thoughts and beliefs (Glesne, 2006). In addition, the student’s work was presented to them for reference during member checking.

## **Peer Debriefing**

Peer debriefing has helped add validity to the study (Creswell & Creswell, 2018). Having a colleague, fellow student, or other professional review and ask questions has provided me with the opportunity to consider different perspectives (Bloomberg & Volpe, 2012; Creswell & Creswell, 2018; Tracy, 2020). These outside perspectives have allowed me to make amendments that would not have been noticed without peer feedback (Shenton, 2004). Finally, I have had my dissertation chair and committee members critique my findings to help solidify my research.

## **Rich, Thick Description**

To maintain rigor, it was essential that, as the researcher, I had fidelity with the course and its students. Peter Mahaffey (2015) reminds us that to be effective in the field of chemistry education, one must understand the students. Objectives and goals should be developed with these students in mind. In my research, that meant “understanding the community members’ slang and inside jokes” (Tracy, 2020, p. 271) along with the verbiage of the novice chemistry student used to explain complete chemical processes. For this study, it meant understanding how students referred to concepts in their non-scientific terms or language and taking the time with the participants to ask for clarification of context. This helped add to the rich, thick description of the qualitative data. This rich, thick description helped create a picture for the reader of the setting and participants, adding to the credibility of the theme development (Creswell & Creswell, 2018).

### **Plan for Sharing and Communicating Findings**

Stakeholders include administration, parents, student participants, and department chemistry teachers. Stakeholders that gained the most from the findings of this action research are Chemistry 2 Honor participants and other chemistry teachers in the department. Findings were shared with participants once the unit ended as an open forum in class to ensure that interpretations of discussions and interviews were correct. Findings were also shared informally with other chemistry teachers during a district professional learning community meeting. The identities of participating students were protected by randomly assigning participants numbers. Sharing these findings with stakeholders has also created an opportunity for suggestions on the direction of implementation in Chemistry 1 courses and future research.

## CHAPTER 4

### ANALYSIS AND FINDINGS

The purpose of this action research was to assess how the use of 3D MolView virtual models influenced high school students' ability to use the symbolic and submicroscopic representations to accurately explain and complete chemical reactions, specifically the reaction mechanism for Fischer Esterification in a Chemistry 2 Honors high school course. Using 3D representation as an innovation to this lesson may help students understand the reaction mechanism better by creating a better connection between 2D symbolic drawings and 3D subparticulate virtual models allowing students to create higher quality short response verbal explanations and written responses. The guiding research questions were as follows:

**RQ1:** How does students' ability to complete a reaction mechanism change after using 3D models to explore the symbolic and subparticulate representational levels of chemistry?

**RQ2:** How do students articulate the process of a reaction mechanism after manipulating 3D virtual models? and

**RQ3:** What is the students' perception of using 3D models to learn a chemical reaction?

Data was collected from the entry point knowledge check, pre-post assessment, and an interview. After the post-assessment, students' articulation of the reaction was assessed to capture quantitative data by quantizing qualitative information from the

student. These findings are presented next, first, the quantitative followed by the qualitative analysis.

### **Quantitative Analysis and Findings**

Quantitative data was collected from a pre-post assessment and by scoring four student interviews on their ability to accurately explain the reaction mechanism. The pre-post assessment was chosen to determine if gains were made in students understanding after the lesson was completed using the innovation.

In this section, the quantitative results from the entry point knowledge check, pre-post assessment and articulation are presented. The following topics will be discussed next: (a) participant selection, (b) entry point knowledge check analysis, (c) pre-post assessment, and (d) articulation analysis.

#### **Participant Selection**

While ten students were present for the orientation, nine students completed all data collection components ( $n = 9$ ). One student was not able to participate in the study because the student was not able to finish the school year in person. Purposeful sampling was used to identify voluntary participants that were qualified for this study (Creswell & Creswell, 2018) to complete an entry point knowledge check, pre-post assessment, whole, small, and independent practice, and an interview after the final unit assessment.

#### **Entry Point Knowledge Check Analysis**

This section concerns the entry point knowledge check given alongside the pre-assessment. These 13 questions determined students' prior knowledge before beginning the unit for this study. The following sections present the reliability testing and descriptive statistics.



### ***Reliability Testing***

***Kuder-Richardson 20 (KR-20).*** Reliability testing for the 12-item entry point knowledge check on functional groups and electron density was below 0.70,  $\rho_{KR20} = 0.45$ . This indicated that internal consistency reliability was lacking potentially due to a small sample size.

### ***Descriptive Statistics***

This entry point knowledge check helped determine if students were ready for the upcoming concepts in the unit of esterification. The participants earned a high score in items related to all objectives but one – identifying functional groups,  $M = .52$ ,  $SD = .50$ . While naming the functional group is a practice of memorizing a pattern on bonded atoms, it did not affect their ability to discuss electron density and its role in reaction mechanisms as previously thought. Identifying the functional groups was thought to be important information to know before beginning this unit. As shown in Table 4.1 below, this item had the lowest mean score. In the articulation assessment, knowing the names of the functional groups did not hinder their ability to describe how these features behaved. In a future study, more careful assessment of what prior knowledge is necessary would be needed. This entry point knowledge check did indicate knowledge of high and low electron dense regions and students were able to apply this in their articulation assessment. Below is an alignment table (see Table 4.1) for the objectives, content, mean and standard deviation for the entry point knowledge check.

Table 4.1 Prior Knowledge, Objectives, Mean and Standard Deviation Alignment Table

Objective	Prior Knowledge	Number of Items	Item Number	<i>M</i>	SD
Students will be able to compare relative electronegativities of sets of atoms	Identify the high or low electronegativity from a pair of atoms- nonmetals	2	1, 2	0.78	0.43
Students will be able to distinguish between three functional groups.	Identifying functional groups (carboxyl, carbonyl, hydroxyl)	3	3-5	0.52	0.50
Students will be able to distinguish between three classes of compounds	Identify classes of compounds (alcohol, ester, carboxylic acid)	4	6-9	0.78	0.42
Students will be able to calculate the FC of an indicated atom	Calculate FC	2	10, 11	0.89	0.32
Students will be able to predict areas of high and low electron density	Identify areas of high and low electron density	1	12	0.89	0.32

### Pre-post assessment

Four open-ended esterification reaction mechanism questions made up the pre-post assessment. These questions were given before the unit began, after explaining the study. They were part of the teacher generated Entry Point Knowledge Assessment, listed as items #13-16 in Appendix A. The following section contains results on (a) interrater reliability, (b) descriptive statistics, and (c) statistical analysis.

### ***Interrater Reliability Value***

***Interrater reliability value.*** A second content area expert and I went over the rubric first. We scored the students' work then reviewed our scores to assess discrepancies in scoring. There were discrepancies in whether to take points off for

missing carbons within intermediates. It was decided not to do so as missing carbon atoms reappeared in the product. Another point to this decision is that in class, we often left parts of molecules off as a shorthand. Students may have been repeating the process used in class which never affected the outcome of the product of the reaction mechanisms. Cohen's Kappa was used for reference and its value is  $k = .932$ . This indicates high reliability of the scoring. Inconsistency of scores were further discussed until we both agreed on the final student scores.

### ***Descriptive Statistics***

Criterion for the product required an accurate symbolic representation of the product, electron pushing formalism required that students place the arrows in the correct placement, formal charge required that students accurately identify atoms that need a formal charge and that it is calculated correctly and finally, the intermediate criterion required the placement of the correct intermediates between the reactants and products. Each criterion was scored on a one to five scale, so each question was worth 20 points for a total of 80 points.

One participant was an outlier in their post-assessment. Removing this outlier, the standard deviations are Post FC (SD = 5.21), Post electron pushing formalism (SD = 3.07) and Post Inter (SD = 2.62). While this further indicates better overall progress in these criteria, this data also highlights the limitations of a small sample size.

The table below, Table 4.2, shows the median scores for each criterion.

Table 4.2 Median Scores for Pre-post assessment Questions

Subscale	Median	$M$	SD
Pre-Product	8.00	7.33	1.41
Pre-Electron Pushing Formalism	4.00	5.33	2.00
Pre-Formal Charge	4.00	4.78	1.56

Pre-Intermediate	4.00	4.00	0.00
Post-Product	20.00	18.56	2.07
Post-Electron Pushing Formalism	13.00	13.22	6.20
Post-Formal Charge	19.00	15.56	6.50
Post-Intermediate	20.00	16.44	6.63

The descriptive statistics for the pre-post assessment indicate a meaningful difference in the pre-post assessment and that a statistically significant change took place due to the innovation.

### ***Inferential Statistics***

***Wilcoxon Signed Rank Test.*** Once results came in for the pre-post assessment, Wilcoxon signed rank test was used because  $n < 15$ ,  $n = 9$ . A Wilcoxon signed-rank test showed that using MolView during the lesson elicited a statistically significant change in students understanding of the reaction mechanism (see Table 4.3). The analysis indicates that using MolView significantly improved ( $\alpha = 0.05$ ) students understanding of a chemical reaction in product ( $z = 2.69$ ,  $p = .007$ ), electron pushing formalism ( $z = 2.31$ ,  $p = .021$ ), FC ( $z = 2.55$ ,  $p = .011$ ), and intermediate ( $z = 2.59$ ,  $p = .010$ ). The effect size values were close to  $r = 1$  (product  $r = 0.95$ , electron pushing formalism  $r = 0.66$ , formal charge  $r = 0.82$  and intermediate  $r = 0.86$ ), indicating a significant effect of learning between the pre-post assessment.

Students were most familiar with the product of this reaction as indicated by  $p = 0.007$ . Gains were made in electron pushing formalism. However, individual scores do indicate that it was understood and accurately applied to all four open-ended short response questions or consistently poorly applied to the questions. The prior-knowledge assessment indicated that students were able to calculate formal charges when given the structure. Students scored low in the pre-assessment in this area as they did not know

what the intermediate structures were and therefore could not calculate a formal charge. After the intervention, significant gains were made in the post-assessment ( $p = 0.01$ ) because they were able to determine the intermediate structure ( $p = 0.01$ ) and apply formal charges as needed.

Table 4.3 Wilcoxon Signed-rank Test Result

Subscale	W	z	p	r
Product	45.00	2.69	0.007	0.95
Electron Pushing Formalism (EPF)	42.00	2.31	0.02	0.66
Formal Charge (FC)	44.00	2.55	0.01	0.82
Intermediate	44.00	2.59	0.01	0.86

<sup>a</sup> The variance in Intermediate is equal to 0

### Articulation Assessment

After the post-assessment, students were asked about their process in solving the reaction mechanisms for the post-assessment. Students' ability to master the language is the start of understanding the concepts and various levels (Stieff et al., 2011). While looking at their work on the recording device and their original work, they were asked about intermediate, formal charges, and electron pushing formalism to obtain the product of a reaction mechanism. Some of the questions were teacher developed and others originated from Bongers et al. (2019) and Bongers et al. (2020) to establish validity. These questions were modified to address the atoms in this reaction mechanism. The following section presents the descriptive statistics for this measure.

### *Descriptive Statistics*

The mean and standard deviation by criterion is presented below in Table 4.4.

Table 4.4 Mean and Standard Deviation per Criterion

	<i>M</i>	SD
Reaction Mechanism Explanation	2.00	0.00
Reaction Mechanism Theory	1.83	0.41
electron pushing formalism Explanation	2.00	0.00
electron pushing formalism Theory	1.83	0.41
FC Explanation	1.83	0.41
FC Theory	1.83	0.41

Overall, students were able to articulate the reaction mechanism and theory used to explain the reaction mechanism well. All students had a clear understanding and articulation of the function of a reaction mechanism and how electron pushing formalism is used to communicate that information. All students scored a two or one for the other criteria, performing very well in their ability to address how formal charges can be used as indicators to determine electron pushing formalism to explain a reaction mechanism. The mean and standard deviation for the overall scores by concept articulated is shown below in Table 4.5.

Table 4.5 Mean and Standard Deviation per Concept

	Mean	SD
Reaction Mechanism	1.92	0.29
electron pushing formalism	1.92	0.29
Formal Charge	1.83	0.00

### Qualitative Findings and Interpretations

Interviews were used to gather qualitative data from the perspective of the participant and served as “night-vision goggles” (Rubin & Rubin, 2011, p. vii). Semi-

structured interviews allowed a flexible interview protocol that invited additional discussion based upon participant responses (Tracey, 2020), a method which proved to be fruitful. The semi-structured interview yielded alternate questions to further gather information provided by participants not considered in the development of the interview protocol (Mertler, 2020) of this mixed methods study. Students were interviewed once, one at a time, after the unit had concluded. The following sections will detail (a) qualitative data sources, (b) qualitative data analysis, and (c) the presentation of findings.

### **Qualitative Data Sources**

Students participating ( $N = 6$ ) in the interview were interviewed in no predefined order. Of the nine participants in the study, six were interviewed. The interview ended once approximately six weeks had passed from the post-assessment. Due to time constraints in the school's schedule, anticipated and unanticipated school events (testing/assemblies), administrative duties, and student absences due to illness, only six of the nine participating students were interviewed. The decision was made to stop interviews after approximately six weeks had passed from the post-assessment. It was evident during the last interview that their memory of the activities, sequence of events for the lesson, and performance results were fading as demonstrated by Sammie, "the red and the blue [3D MolView filter] showing; I can't remember if it was electron density or electronegativity at this point because of the oxygen...I can't remember at this point. But that was pretty useful..." and Bec, "I kinda forgot what grade I got on this."

Of the students interviewed, four were boys and two were girls. Three participants were seniors and 18 years of age. The other three were 17-year-old juniors in high school. All had been identified as gifted and talented by the state prior to entering high school.

Four of the six were participants in the school's STEM program. All participants were Caucasian.

### **Description of Qualitative Data Analysis**

Interviews for qualitative data took place after the post-assessment, during regular class time, at a table next to the door in the hallway. During the one-on-one interviews, participants were asked questions about their experience with the unit, the content, and using MolView. The one-on-one interviews allowed me to hear the students' experience with the unit and using MolView in their own words. Listening to the interviews, I was able to hear how they connected types of representations and content, what components of the lesson were helpful, and if they used MolView as an aid or other strategies.

The interviews were recorded using Screencastify which allowed the student and me to refer to their work as needed for clarification. Screencastify is a screen recording Chrome extension approved by the district. The videos were converted to .mp3 files from Screencastify and entered into Happy Scribe for transcribing.

Happy Scribe is online software that transcribes recorded data one of two ways, automatically or by human review. The automatic transcribing feature was used taking minutes per video. However, once the transcriptions were generated, I spent a week listening to them again to check for grammatical errors, such as spelling or homophone confusion and to improve accuracy.

From Happy Scribe, transcripts were downloaded to MS Word Documents, then Delve to begin the first cycle of coding. Delve is online software used to analyze qualitative data. Interviews can be uploaded and coded within Delve and further organized for analysis as shown in Figure 4.1.



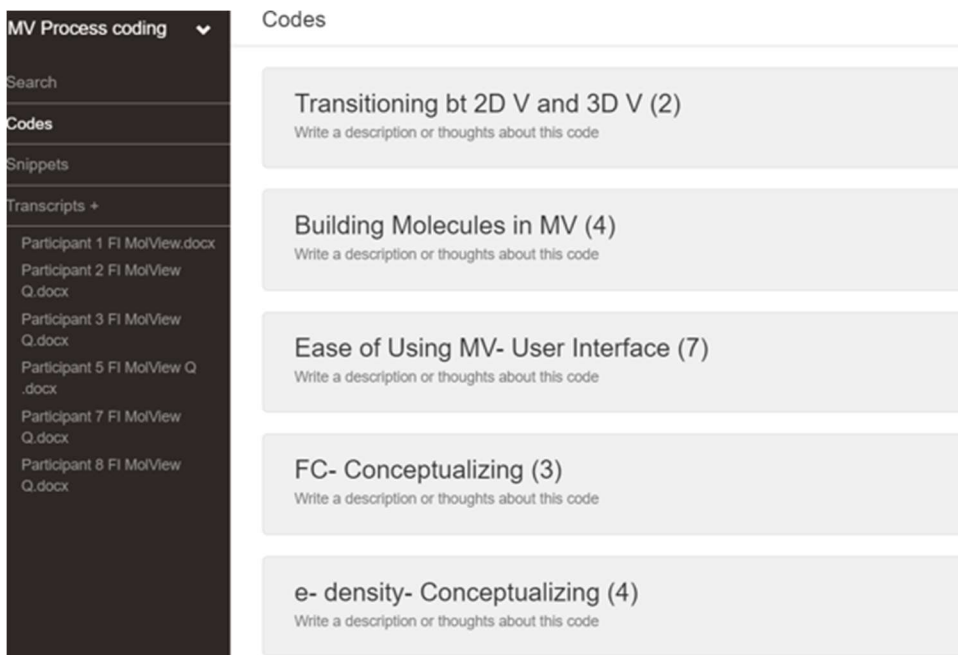


Figure 4.1 Screenshot of Delve Process Code Project

During first cycle coding, I frequently went back to Happy Scribe and replayed the in-sync video and transcription (see Figure 4.2) to confirm what part of a reaction or molecule was being referenced and added these notes to the Delve transcripts.

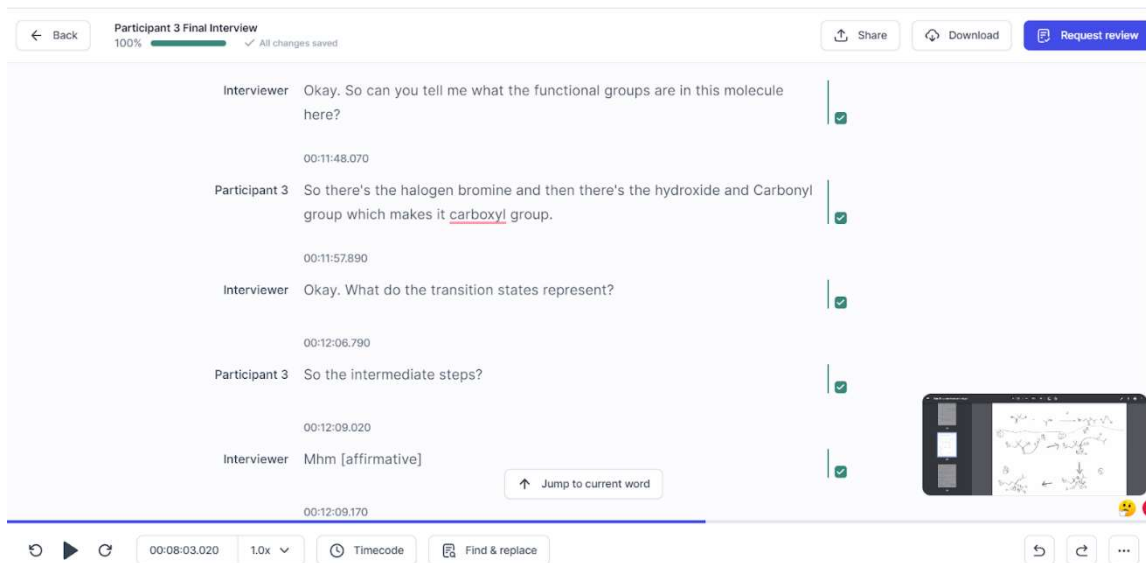


Figure 4.2 Confirming Context of Interviews Using Happy Scribe

From here, the process of inductive analysis began. Inductive analysis is the process of distilling data to find relationships that may even seem unrelated to synthesis

new overarching themes. Phrases and sentences were analyzed from the transcribed interviews to identify salient features of the students' understanding and experience. Codes were generated from these segments to provide meaning to the data (Vogt et al., 2014). These were further synthesized into noteworthy pattern codes that offered meaning to their experiences and the impact of the innovation. These codes were further summarized into categories to generate themes that concisely explain the key features of the qualitative data. Themes were the culminating product of the iterative process of grouping and regrouping related data, the process of coding (Tracy, 2020). The inductive analysis made impactful features of the unit and innovation apparent and brought to light aspects of the unit design that were not considered during the planning or conducting of the study. These themes became the foundation of a framework constructed from the findings of the study (Johnson, 2008). Here, qualitative inductive analysis was used as a method of “systematically organizing and presenting the findings of the action research in easy that facilitate the understanding of these data” (Parsons & Brown, 2002, p. 55).

Coding is a method of qualitative analysis that “calculates meaning” (Saldaña, 2016, p. 10). Meaning is calculated (Saldaña, 2016) through a process of discovery that leads to other discoveries (Fuller & Goriunova, 2014) from which the corpus of data is reconfigured to find broader themes and assertions (Saldaña, 2016). In this study coding was used to pull phrases from interviews to interpret students experience with MolView. Each cycle of coding underwent several rounds to determine how to best represent the data, the participants and respond to the research question. It required taking care to avoid under and overestimating the value of what the students shared during the interview (Schwalbach, 2003). The iterative process of analysis occurred over five months. Below I

describe my process for qualitative analysis using thick rich description in the following sections: (a) first cycle methods, (b) transitioning to second cycle coding (c) second cycle methods, and (d) theme development.

### **First Cycle Methods**

Individual interviews were analyzed sentence by sentence to determine how students felt about using MolView over two rounds. The methods used for first cycle coding were in vivo coding and process coding. In vivo was used for the first round and process coding for the second round. These methods helped ensure that student voices remained intact and created a picture of the actions that supported student understanding of the reaction mechanisms and the concepts around the reaction over time (Saldaña, 2016).

### ***In Vivo Coding***

Saldaña (2016) indicates that in vivo coding is a means to develop an understanding of a student's experience through the prioritization of their voice. This prioritization was key to enhancing my understanding of the student experience with MolView. In vivo coding was used to capture the language (Strauss, 1987) students use to explain their perception of the innovation during the first round of first cycle coding in Delve. Instructors often overlook how students think about the content (Weinrich & Talanquer, 2016), which in vivo coding helped shed light on the study. In vivo coding allowed me to hear if and how students refer to or between representation levels, content, and their user experience with MolView in their own words (Tracy, 2020). In vivo coding provided insight as to (a) how students felt about using MolView, (b) when

MolView was beneficial, (c) under what conditions and context, and (d) how long it was useful. Test scores alone would not reveal if and why MolView would have been useful.

To do this, Delve was first used to identify in vivo codes for one participant at a time. Before moving on to the next participants transcription, selected proportions were further edited to add context using square brackets using Delve's editing feature, as shown in Figure 4.3, as suggested by Dr. Bice.

Only when the molecules got bigger [in 3D MV did it become difficult to translate] and I had a little bit more to focus on [with the 3D lucent filter on], because it was a little bit difficult to remember what colors corresponding with which atom and how it was oriented. But I felt like if you just looked at it [the 2D virtual molecule] first, I need to be able to see where you are and what you needed to do [to translate the large 3D molecule with lucent filter].

when the molecules got bigger

if you just looked at it first, I need to be able to see where you are and what you needed to do.

little bit difficult to remember what colors corresponding with which atom and how it was oriented

Figure 4.3 Addition of Context in Delve Using Square Brackets

Some sections of interviews had run-on sentences or especially long statements. In these instances, sentences were broken down and multiple codes applied. These sentences were searched for quotes that captured feelings of success, frustration, accomplishments, and understanding of content. For example, Sammie stated “you showed us that [viewing reactants and intermediates in 3D MolView with filter], and I was like, oh, well, maybe [I can predict how reactants will react]. Yeah. So that made it a little bit easier.” This was assigned the in vivo code of “teacher modeling.” This statement exemplified that the whole group guided practice served as a model of how to “read” subparticulate models and apply them to symbolic representations. Charlie stated “I knew about the electronegativity but seeing it in [3D with a colored filter in MolView] the molecules, like in use, really helped me understand where it's coming in play [in the steps of the reaction mechanism].” This was assigned the in vivo code of “seeing it...helped me understand...” Here, Charlie captures the combining of prior knowledge

from Chemistry 1 Honors recalled and was able to connect it to the 3D virtual models to be applied to the new content. The bulk of the in vivo coding was done over ten days. During this time, notes were made to record initial thoughts on the meaning of what participants were communicating. A total of 195 in vivo codes were made during the first round of first cycle coding.

### ***Process Coding***

After in vivo coding was completed, process coding was used for the second round of the first cycle. A benefit to process coding is that it can help identify (a) routines in behavior (Corbin & Stauss, 2015), (b) actions students took to work out a problem (Saldaña, 2016) and, (c) changes in behavior or thinking over time (Saldaña, 2016). These codes use gerunds and transition words to identify actions of a process (Saldaña, 2016). Throughout the process, notes were made to capture initial thoughts on potential categories and themes in a notebook. All transcripts were entered into a project in Delve. Each transcript was reviewed sentence by sentence for evidence of thinking, actions, and changes. For example, when students spoke accurately about concepts and how they came to understand them using MolView or other activities, these were coded as Conceptualizing. This was further broken into the concept that was conceptualized, such as, Conceptualizing Electron Density. After several reviews with co-advisors, several codes were recoded to indicate active or passive learning. Several process codes were still too broad, however, and appeared more like categories. After several rounds of process coding, process codes were moved to categories and then differentiated further from there. Visualizing became a category which was broken down to identify what students were visualizing. Mental modeling promoted and broke down to identify what students

were imagining and if it resulted from MolView. Once significant data had been identified in Delve, all codes were downloaded into MS Excel then to Google Sheets. From here, process codes continued to be reviewed using A-Z filtered view and find features. Several rounds of process coding were completed well into the transition process and second cycle of coding, taking approximately four months to complete. A total of 75 process codes were developed over time.

### ***Peer Debriefing***

Once in vivo coding was completed, a Delve Project was shared with Dr. Holli Bice and Dr. Tang for peer debriefing. In response, it was suggested to add comments to codes and provide additional context (H. Bice, personal communication, October 10, 2022). After sharing the Google Spreadsheet with data, codes and pattern codes, there was a lot of discussion around the meaning of the codes and clarification of codes. Once categories were developed, Dr. Tang suggested promoting a handful of pattern codes to categories to support a theme. The codes in these newly promoted pattern codes were reviewed and further differentiated. Peer debriefing went over approximately over six to seven months.

### **Transitioning to Second Cycle Coding**

Once I had completed the first round of first-cycle coding, I exported Delve Codes and Transcriptions to Microsoft Word for additional reviews. These were printed and reviewed by hand. They were printed three times for review before beginning the second cycle of coding. During this time, there was a transition period composed of time away from the data and rethinking the data. During this transition period, the meaning of the data and key words were reexamined in a “circular, iterative, and reflexive method”

(Tracy, 2020, p. 220) to fine tune word usage and rephrase codes as new meanings were noticed over the process of first cycle coding (Saldaña, 2016). Other data was recoded before starting the second cycle because they were found to have more similarity with other codes than originally thought (Saldaña, 2016).

From Delve, additional context, codes, and code reassignment or further decomposition was made three times by exporting the Codes to Microsoft Excel and then a Google Sheets Spreadsheet (Sheets) in the transition process. The data and codes for in vivo and process coding were then copied into a single sheet (see Figure 4.4).

1	Participant	Data	Code
2	Participant 7 FI MolView Q.docx	t took all of chem 1 and all of the electron and molecular geometry that we learned from there and, like, applied it to the molecules and applied it brought in formal charge	Activating prior knowledge
3	Participant 2 FI MolView Q.docx	But from the very beginning, where it was just moving stuff around through resonance and instead of, like, solving exactly what's going to happen and why [reaction mechanism], whenever you're introducing two things together, that was the part that was difficult for me, but I ended up getting it down at the very end.	Struggling with translation
4	Participant 1 FI MolView.docx	<i>2D, 3D and stuff like that. But kind of understanding it was more difficult.</i>	<i>understanding was difficult</i>
5	Participant 2 FI MolView Q.docx	It [using MV] gets to a point where it's [the molecule is] not really decipherable, but on a smaller scale, you can still read it [the molecule in 3D].	limitations of using MV
6	Participant 2 FI MolView Q.docx	<i>2D drawn models, you can kind of just look at it and you'll just see, like, a swamp of just things, and you don't know what's going to go anywhere</i>	<i>don't know what's going to go anywhere</i>

Figure 4.4 Screenshot of Google Sheet with Initial Data and Codes

Multiple codes related to cognitive load were split to examine the conditions (an activity or using MolView) that change cognitive load. Patterns that were beginning to emerge included “Learning Strategies” used by students and embedded within the lesson design as well as how students were “Connecting Different Levels of Representations.” While the iterative process did not end here, this was a cleanup process before the second cycle coding process began. This transition provided distance and time from the work to return to it with fresh eyes. This step took about six to seven weeks and was revisited frequently after starting the second cycle.

## Second Cycle Methods

The second cycle process is a process for “basic assembly with opportunities for the researcher’s elaboration” (Saldaña, 2016, p235). The coding process was an iterative process in which I continued to make notes in a notebook and changes in Sheets on codes and categories after the first cycle of coding and transition period and into the second cycle. The next step was to assess the first cycle codes to develop smaller groups of information that could be reorganized into categories and themes that paint a bigger picture of the study. Second cycle coding began by adding additional columns in Sheets for Pattern Codes and Categories. The sheet was organized by hierarchy, data on the left and progressed to categories on the right side of the sheet (see Figure 4.5).

1	Participant	Data	Code	Pattern Code	Category
195	Participant 8 FI MolView Q.docx	I like drawing them out before I could ...like on the computer, before I wrote them down so I could see what was going to be interacting with each other, because that's whenever I was still learning and seeing what was happening and getting the pattern down,	Self-correcting/self-checking tool	checking subparticulate to complete reaction mechanism	Reference mode mechanism
196	Participant 7 FI MolView Q.docx	When I was writing this, I feel like I knew exactly what to say.	being prepared	Feeling confident for the test	Self-efficacy abou
197	Participant 8 FI MolView Q.docx	I definitely feel more confident	confident	Feeling confident for the test	Self-efficacy abou
198	Participant 7 FI MolView Q.docx	I felt good	confident	Feeling confident for the test	Self-efficacy abou
199	Participant 7 FI MolView Q.docx	I felt prepared.	being prepared	Feeling confident for the test	Self-efficacy abou

Figure 4.5 Organization of Data, Codes, Categories within Google Sheet

These categories, pattern codes and first level codes continued to be reviewed and reorganized by using the A-Z Sort filter in Sheets to ensure I was connecting the meaning behind the collected data (Charmaz, 2009). The second cycle coding was completed over three months.

### *Pattern Coding*

Pattern coding is a second level code that pulls together more descriptive first level codes to generate broader abstract ideas (Punch, 2014) from which categories were developed. Pattern coding was used to develop categories because it brought together smaller ideas to find patterns in students experience with MolView and the unit. Pattern







At this point, notes on reorganizing pattern codes and codes were made electronically either in the Google Spreadsheet or using a voice recorder on my cellular phone to record later into the Google Spreadsheet. Before major changes were made to a Google sheet, a copy was made to record original thoughts (see Figure 4.8), even though Google automatically saves accessible versions of the Spreadsheet.

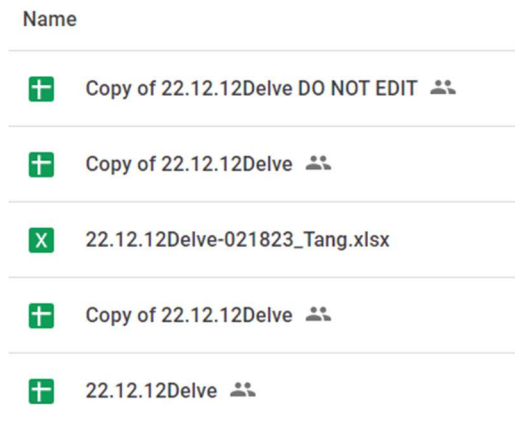


Figure 4.8 Copies of MS Excel and Google Sheet Spreadsheets

Also shown above is a version made and shared by Dr. Tang for feedback directly within the Spreadsheet. These copies were useful because they also created a record of initial thoughts of data, codes, patterns, and categories. Inductive analysis ended with the development of four themes and 14 categories. Theme 1 addressed RQ1, theme 2 addressed research question 1, theme 3 with RQ3, and theme 4 aligns with RQ1 and RQ2. These themes are presented below (see Table 4.6) along with example pattern codes and data.

Table 4.6 Emergent Themes and Categories, Pattern Codes and Data

Theme	Category	Example Pattern Codes	Data Examples
The integration of learning strategies into MolView activities aids student learning.	Optimize learning opportunities with MolView	Ample practice	So, I'd definitely say more was good.
		Spacing practices	I liked that they were spaced out, and not "do these eight for homework" and then never see them again.
			If we did less of it, but we kept it spaced out, I think I probably would have been okay, just as good.
	Accounting for cognitive load when designing course activities	MolView group activity created cognitive load	It's just kind of tedious [to capture intermediates for MolView group activity] and so I think I just referred back to this kind of drawings [2D drawings, self-made for reaction mechanisms].
			But it [MolView group activity using MolView to create a rxn mechanism] was so tedious that I just probably wouldn't do it again unless maybe I was having a really rough time.
			With MolView, I found it hard to make steps.
		2D virtual models reduce cognitive load	2D models, it's a lot more straightforward and can see it all in one spot super easily
			But I feel like using MolView as an introduction to it [EPF] was much more helpful to see the 2D model.

	Group discussion	Subparticulate level	After discussing electron density and formal charge, like, depending on the atom, it was a lot easier to see.
		Reaction mechanisms	We were able to discuss it most of the time afterwards, especially discussing it with our peers
			Going through it [MolView Group Activity] and talking about electronegativity and lone pairs and formal charge, those things, going through that and thinking through it and then using it really helped to make sure I actually understood
	Teacher-guided practices	Activating prior knowledge	All the preparation and background work that we did, that helped a good bit
			It took all of Chem 1 and all of the electron and molecular geometry that we learned from there and, like, applied it to the molecules and applied it brought in formal charge
		Teacher modeling how to use MolView	Doing it together as a class helped me understand more of, like, some of the extra features that I may not have noticed
MolView facilitated students' conceptual understanding.	Understanding concepts by creating mental models	Creating mental models of concepts	Dedicated class to learning how to use it
			Able to see how the different sites can react with each other was helpful.
			I visualize the molecules, I kind of do it in a 2D visualization with the lucid structure because it's just

		easier to wrap your head around that as just one thing
	Understanding other symbolic representations	Yeah, that [3d] would help with that [dash wedge models].
	Understanding the subparticulate to determine the symbolic	Going through the steps, I was thinking about where the... I was visualizing the colors of the MolView onto the paper
		I was actually able to envision, oh, this is really blue right now. This is why it's attacking. That's why there's a nucleophilic attack
Learning concepts by visual representation	Visualizing the subparticulate level to determine the symbolic	3d structure and then the mapping out of the electron density so that helped visualize where stuff is more likely to react and bond
		The 3D view, it would show you the higher and lower electron density regions because formal charges based off of the same thing, higher and lower electron density regions, you can directly visualize what an area would even look like
	Visualizing the subparticulate level	You can see where you can see where there wouldn't be electrons and where there would be more electrons
		3D MolView model] helps me realize how much of an impact it [formal charge] has
	Visualizing the symbolic with	It [MolView group activity] was helpful because with that 3d slide,

		the subparticulate	like you mentioned, it was nice seeing how it changed.
			I knew about the electronegativity, but seeing it in the molecules, like in use, really helped me understand where it's coming in play
	Understanding the reaction mechanism	Applying concepts to new reactions	I was going to learn a new reaction mechanism, I would look at the reactants before in MolView to see where the reaction sites are going to be
		Understanding the reaction	In the beginning it was, but getting towards the end, as I said earlier, once you already had the visual representation understood of where the high electron density areas were and the low electron densities were, it wasn't really helpful to plug the same things in again and look at things that you've already seen before.
Chem ed tools' inherent limitations in dealing with complex matters should be accounted for.	Cautious about cognitive load	Translating large molecules	In MolView, with the two molecules, when you put them in the same screen, that made it harder because you can't really maneuver around with both of those molecules. That made it more difficult
		Supporting cognitive load	I don't think it [formal charges/electronegativity] was more difficult to understand [using MolView]. I don't think it hindered me at all
		Temporary increase in cognitive load	I don't think it was more difficult to understand? It's just the original reading of it at first, but then once you get it down

		Being able to see it [in color]. I mean, at first it's kind of blunt, what are you looking at?
Consider restrictions on what students could do or see	Hindered by not displaying lone pairs	Especially when we're doing transferring slides, we'd have to put the lone pairs on ourself, and that's just a hassle
	Overlook intermediates	If you had to do anything beyond doing that, MolView just isn't capable of doing that.
	Does not allow incorrect structures	It told you what was wrong.
Addressing student preference towards models	Benefits to all virtual representation	Well, the 2d virtual model, it made it cleaner to look at, but the 3d virtual model, being able to see where higher electron and lower electron density [lucent filter] area fell, that was really helpful.
	Preferring 2D Virtual Models	Easier to just get the 2D version [virtual] going
	Benefits of 3D virtual modeling	With the 2D, it's hard to see the electron density.
Support learning different representation levels	Translating between 2D and 3D	With the smaller molecules and just one, it was pretty easy to get
	Connecting multiple levels	I think it would have helped me kind of solidify seeing another way to represent it.
	"Intuitive layout"	It was pretty intuitive with all of the controls and stuff like that.
	Easy to make molecules	It was never difficult. It was really easy to use. It was really easy to get a hold of and to continue using



			MolView wasn't difficult in making a molecule and viewing a molecule
MolView served as reference resources for students to track learning progress and performance.	Self-evaluation of 2D hand drawn models	Quick 2D generation	My handwriting is just that bad. So that's when the 2D [MolView] comes in handy
		Self-checking 2D hand-drawn structure	Whenever we made the slideshows [MolView group activity], like when we had to do step by step slideshows, then it did [help determine if molecule was correct].
	Verifying subparticulate levels for a reaction mechanism	Starting the reaction mechanism	On the computer, before I wrote them down so I could see what was going to be interacting with each other
			If I forgot what was happening it would kind of remind me
		Checking subparticulate to complete reaction mechanism	I was still learning and seeing what was happening and getting the pattern down, so being able to see where things were going to happen.
			I would [go to MolView if I was having a really rough time],
		Checking concept understanding	It [MolView] adds an extra layer of like not a set of support [when learning about EN the first time in Chem 1], but kind of support just so you can fall back on
	Self-efficacy about their performance	Feeling confident for the test	I felt prepared.

Making progress over time/practice	So, I'm not gonna lie and say it was good from the start, it was really bad in the beginning, but it got better and better.
Virtual models increasing interest in the topic	I thought it was really cool [3D rotation of molecules] because you can't do that on paper, so I thought it was really cool and I liked seeing stick out [3D virtual molecule].

---

### Theme Development

#### **Theme 1: The integration of learning strategies into MolView activities aids student learning.**

This theme defines the need to incorporate multiple learning strategies with MolView. It is significant because MolView would not have been effective alone. Using discussions, small group practice, guided practice, teacher-modeling while accounting for cognitive load, activities can be built around the use of MolView to support students' understanding of the symbolic reaction mechanism and the subparticulate properties explaining the mechanism. Categories making up the theme on the learning strategies around the usage of MolView are (a) optimizing learning opportunities, (b) accounting for cognitive load (c) including group discussions, and finally (d) starting with teacher-guided practice.

#### ***Optimizing Learning Opportunities***

Optimizing learning opportunities is defined as providing small volumes of spaced practice after being oriented with MolView and the reaction mechanism. Consistent exposure over time with domain-specific knowledge allows students to move

information from working memory into long-term memory (Chase & Simon, 1973; De Groot, 1965). Bec's statement below reflects her perceived effectiveness of the method:

Bec: [I] liked that they [the practice] were spaced out, and not "do these eight for homework" and then never see them again

Jon: Doing it every day would allow less time to forget and take it from a step back, take two steps forward instead to keep going...I think that if there was more [practice in a day], it would have gotten to the point where it would just bog you down, and by the end of it, all the practice problems would just kind of get annoying

Charlie: I definitely think spreading it out over the four days is better [than all of the practice in one day.]

All participants felt that the spacing of the practice and completing only three per day with a review was beneficial to their learning.

### ***Accounting for Cognitive Load***

This category is defined as the change in cognitive load throughout the unit due to how and when MolView was used. A side-by-side configuration of information maximizes working memory to translate between models (Kirschner, 2019). Having students hop between programs slowed students down and created some frustration because MolView could not create all of the symbolic features (such as lone pairs of electrons and electron pushing formalism arrows) I required from the activity. This was represented in Bec's statement of "it was helpful. It was just very tedious taking all the screenshots of every single step [of the reaction mechanism for the MolView Group activity]." However, participants still found it useful because the activity pulled together

the symbolic and subparticulate levels of content Bec stated “[the MolView Group activity] was helpful because with that 3D slide [of the intermediate steps of the reaction mechanism] ...it was nice seeing how it [3D lucent filtered intermediate steps] changed [throughout the reaction mechanism].” MolView’s 2D virtual representations did seem to minimize increases in cognitive load. Students indicated that the 2D virtual models supported their learning progress. Charlie said, “2D models, it's a lot more straightforward and can see it all in one spot super easily” and Gracie said, “But I feel like using MolView as an introduction to it [electron pushing formalism] was much more helpful to see the 2D model.” Students were able to think more about the concepts and how to apply them and less about how to draw the structures and interpret the representations.

### ***Including Group Discussions***

This category is defined as using group discourse to aid students’ understanding. To develop conceptual understanding, discourse amongst pairs has been proven beneficial (Aldahmash & Abraham, 2009; Rodriguez & Potvin, 2021). While the MolView Group Activity required a partner, students had the option of completing all other practice work independently or with a small group. Gracie stated “after discussing electron density and formal charge, like, depending on the atom, it was a lot easier to see” and Bec concurred with “Yeah, like making [2D virtual reaction mechanism] the steps and speaking out loud [during MolView Group Act]” helped him understand the reaction mechanism. Over the unit, all students checked in with a partner and most did their daily bellwork practice with a partner or small group.

### ***Starting with Teacher-Guided Practice***

Teacher-guided practice is defined as providing an instructor-led introduction to MolView before beginning the chemistry concepts by activating prior knowledge as a whole group. The combination of visual and aligned verbal instruction increases the effectiveness of working memory and likelihood storing the information into long-term memory (Caviglioli, 2019). Students were guided with verbal instructions that matched the visuals presented on the SmartBoard. Before introducing MolView in the context of a reaction mechanism, the idea of using colors to represent the property of temperature changes across the globe was reviewed through probing questions. Sammie stated that “all the preparation and background work that we did, that helped a good bit.” Then, the instructor-led introduction to MolView guided students through several features of MolView as a whole group followed by students building a molecule on their own and having it checked for accuracy. Charlie indicated “doing it together as a class helped me understand more of, like, some of the extra features that I may not have noticed,” and Gracie stated in the interview that “I would have been much more confused as to why it [the reaction mechanism] was happening. But I feel like using MolView as an introduction to it was much more helpful.” There were many facets to account for when implementing a chemical education technology tool. Teacher-guided practice with the tool and content was one method to minimize the likelihood of misinterpreting the model which leads to developing and reinforcing misconceptions.

### ***Summary***

All students addressed components of how the lesson was designed in combination with the usage of MolView. Evidence is clear that the design and structure

of activities within the lesson and for the implementation of virtual models were perceived as impactful by students.

**Theme 2: MolView facilitates students' conceptual understanding around a reaction mechanism.**

This theme defines the ways that MolView aided students' understanding of the symbolic level reaction mechanism and subparticulate level electron pushing formalism and formal charge. Mental models are unobservable representations of a concept (Bongers et al., 2019; Chittleborough & Treagust, 2007; Johnstone, 1993) which can be made observable by creating a visible representation of the mental model. It is not until students either discuss the mental models they use or visually represent their model that instructors develop an understanding of how students use the subparticulate and symbolic representational levels to explain the reaction mechanism. Bongers, Northoff and Flynn (2019), Bhattacharyya, (2014) and Galloway et al. (2017) remind us that students learning reaction mechanisms are adept at identifying and repeating patterns by focusing on surface level features of the symbolic level (the hand-drawn reaction mechanism) without using the subparticulate level (properties such as electron density and formal charge) to fully explain the reaction mechanism. MolView's 3D virtual models helped students create a mental model to visualize why a reaction mechanism follows the steps it does. All students in this study referred to the visuals they saw in MolView and used them to create their own mental model to apply to the reaction mechanism they were working through. This suggested that new or modified schema of electron density was developed and the 3D MolView served as a cue that moved information from sensory, to working then long-term memory, making it available for use later (Bongers et al., 2019;

Neumann & Kopcha, 2018; Northoff, & Flynn, 2019) This theme was built around the following categories, (a) understanding concepts by creating mental models, (b) learning concepts through visual representations, and (c) overall understanding of the reaction mechanism.

### ***Understanding Concepts by Creating Mental Models***

This category is defined as students' understanding of symbolic and subparticulate representations, their relationship and concepts resulting from the mental models that students developed from working with MolView's 3D virtual models. While students often rely on pattern recognition to complete a reaction mechanism and omit the subparticulate explanation (Bhattacharyya, 2014; Bongers, Northoff & Flynn, 2019; Galloway et al., 2017), the students in this study articulated their understanding of how the subparticulate properties, like electron density, are indicators to completing the symbolic representation of a reaction mechanism. Bec stated, "I was actually able to envision, 'oh, this is really blue right now. This is why it's attacking. That's why there's a nucleophilic attack,'" while Gracie said, "I was visualizing the colors of the MolView onto the paper." While students articulated their understanding, they all tried to discuss concepts we had discussed and seen in MolView. It was evident in their interviews and articulation that they were able to imagine representations of these concepts upon the molecule.

### ***Learning Concepts Through Visual Representations***

This category is defined as students understanding the subparticulate, symbolic levels and their relationship because they were able to see the 3D virtual representations. This was first in part due to students' ability to translate between their 2D hand-drawn

structures, 2D virtual and 3D virtual structures which moved information to their long-term memory (Kirschner et al., 2018) and helped students develop explanations between the two (Suits & Sanger, 2013; Suits, 2015). Aston describes that the “display, it kind of helped me understand where the electrons were focused,” while Sammie commented “it helped show where the bonding would be,” and Aston said they liked being able to “able to see where things were going.” The 3D virtual representations subparticulate properties such as electron distribution (see Figure 3.4) or charges on the molecule helped students further conceptualize the concept. These concepts moved from being notations on a 2D structure to fully developed construct.

### ***Understanding the Reaction Mechanism***

Understanding the reaction mechanism is defined as students having conceptualized the reaction mechanism not only at the symbolic level, but at the subparticulate level and no longer needing to refer to MolView. Interviews and articulation suggest that students had developed a strong conceptualization of the process and would apply MolView to learn a new reaction mechanism. . For example, Jon stated,

You'd see the pattern and then you see the logical steps that led to that pattern, and then you can apply those going further [to new reactions]...if I was going to learn a new reaction mechanism, I would look at the reactants before in MolView to see where the reaction sites are going to be.

All students indicated that once they were comfortable with the reaction mechanism, they no longer used MolView as students were guided at the beginning of the lesson. Charlie said, “near the end, I had already begun to understand it, and at that point, it became more



of a hindrance because you have to set up the molecule.” This was evidence that students had reconciled the 2D hand-drawn symbolic representations with the new subparticulate level concepts represented in MolView’s 3D virtual representations.

### ***Summary***

All participants discussed the visualizations from MolView and implied the formation of their own mental models during the interview and during the articulation assessment. As a result, the combination of the 3D visual images and the formation of mental models, students developed a full understanding of the reaction mechanism and therefore the ability to articulate a reaction mechanism at both the symbolic and subparticulate representational levels.

### **Theme 3: Chem ed tools' inherent limitations in dealing with complex matters should be accounted for.**

Virtual chemistry education tools are defined as technology that supports learning chemical concepts (Al-Balushi & Coll, 2013; Antonoglou & Sigalas, 2011; Barrett et al., 2015; Stull et al., 2013). These tools can provide students with powerful learning experiences under the right circumstances. Students in this study indicated directly and indirectly that design features contributed to their understanding and hindered their progress. For example, all students interviewed stated difficulties translating between the 2D virtual models and 3D virtual models when (a) it was a large molecule with many atoms and (b) there were two molecules built on the screen, even though building the molecules in MolView was “easy” due to its “intuitive” design, according to all participants but one. While not all students preferred the virtual molecule to complete the reaction mechanism practice, all participants appreciated the option of various choices

and filters provided in MolView. One drawback to the online software, according to half of the six interviewed participants, was MolView's lack of ability to place lone pairs of electrons and use electron pushing formalism arrows to create the reaction mechanism or a resonance structure. Collectively these main ideas define this theme with the following four categories indicating that its design should be, (a) cautious with cognitive load, (b) considerate of restriction around what students can or cannot see, (c) address student preferences in models, and (d) support learning different representational levels.

### ***Caution Around Cognitive Load***

This is defined as being aware of cognitive load inherent in the design when selecting chemical education technology tools. Animations and 3D virtual models can help move new concepts into long-term memory, but this requires that the new virtual models be similar to models' students have been working with. For students to translate new models, the new models must have features, such as coloring or shapes, which are similar to prior models that students are familiar with. This creates a bridge constructed from existing schema for the new content to move from working memory to long-term memory (Williams & Clement, 2015). Chen et al. (2017) indicate that unfamiliar features will distract students, resulting in an increase in cognitive load, a factor that inhibits learning (Rop et al., 2018). This did occur as stated by Gracie, "being able to see it [in color], I mean, at first it's kind of blunt, 'what are you looking at?'" All participants indicated having difficulty in reading and moving large molecules and when two molecules were on the screen as indicated by Charlie: "...in MolView, with the two molecules, when you put them in the same screen, that made it harder because you can't really maneuver around with both of those molecules. That made it more difficult," and

Jon “Whenever a molecule gets really big, to the point where you're just looking at it and you see like a whole bunch of random colors everywhere. It gets to a point where it's not really decipherable.” Bec stated “I don't think [formal charges/electronegativity] was more difficult to understand [using MolView]” indicating that overall, participants did not perceive MolView as hindering their understanding.

### ***Consideration of Restriction Around What Students Can or Cannot See***

This category is defined by considering the restrictions around molecular properties when selecting a chemical educational technology tool. While MolView was specifically chosen for its simplicity, to minimize cognitive load effects, and its side-by-side view of model, to account for dual coding, Bec, Jon and Sammie wanted a more complicated molecular building program. They felt that to meet the needs of the assignment and to further aide their understanding of a full reaction mechanism, they would have preferred a program that also showed lone pairs on the 2D virtual side and would create multiple models in the 3D side that were easy to view and manipulate. Jon did recognize the limitations to more complicated programs but felt that extra time spent learning to use the program as a whole group would have cut the time required to complete the MolView Group activity. Jon stated,

[It would have been more] beneficial to have a more complicated but more capable platform and... dedicated class to learning how to use it... [a program] that had what MolView has plus the ability to notate reactions or resonance, that would be a lot better for trying to use technology to learn resonance structures and the esterification reaction mechanism.

He described MolView as a prototype. Gracie and Aston recognized and appreciated the boundaries set by MolView; Aston stated, “if you put the wrong central item and it wouldn't build it at all 3D because it would say ‘this molecule is overloaded.’” It is a careful balance when selecting chemical educational technology between representations that are too simplified or complex. This must carefully be determined based on the capacity of your students and the time available to learn the technology.

### ***Address Student Preferences in Models***

This category is defined by considering the features available when selecting a chemical educational technology tool. This qualitative data from the interviews suggested that MolView did help all participants understand the content. However, students had preferences in models when working out the reaction mechanism practice that was dependent on their level of understanding. Most students preferred using the 2D virtual model or hand-drawn after understanding how to complete the reaction mechanism. Sammie commented that “[the daily practice] got to the point where just the 2D models worked the best for me, and I didn't really have a preference between MolView and me doing it.” Gracie found overall access to the virtual models helpful, saying “I liked being able to have that visual with MolView.” Jon recognized the benefits of both types of models stating “Well, the 2D virtual model, it made it cleaner to look at, but the 3D virtual model, being able to see where higher electron and lower electron density [lucent filter] area fell, that was really helpful,” as did Gracie, who said “I probably liked that [2D virtual] more than the 3D side, but I still like the 3D side in the sense that I was able to move it around and see all the different variations of it.” The variety of models allowed students to learn to translate between them and determine which best suited their needs.

### ***Support Learning Different Representational Levels***

This category defines a user-friendly layout and experience of a chemical educational technology tool as aiding student learning. MolView's design placed the representations side-by-side, a configuration that helps students translate models (Kirschner, 2019). All participants but Bec found MolView easy to make molecules in and had little difficulty in translating between 2D and 3D representations in MolView.

Some quotes include:

Aston: It was never difficult. It was really easy to use. It was really easy to get a hold of and to continue using.

Jon: Viewing a molecule, it was really easy.

Bec: The actual transition itself, like the physical clicking [within MolView], that was nothing.

For these students, MolView was easy enough to make use of its multiple representations and translate them to their work.

### ***Summary***

All participants felt like MolView did not hinder their understanding of subparticulate levels. While four students would have preferred additional features, the design of the activity played a factor in this wish. All participants appreciated the various types of representations and how the types helped support the learning of new content but reinforced prior concepts. MolView's design was appropriate because it did support learning based on where they are as chemistry learners and the objectives of the unit.

**Theme 4: MolView served as reference resources for students to track their learning progress and performance.**

This last theme is defined as how and why students use MolView and the resulting effects. Educational technology has the power to change engagement, motivation, and performance. MolView served as a resource for students to check their work and verify their understanding of concepts and 2D structures. This helped students develop self-efficacy within the content, which further motivated students to move through the unit. The final theme for this action research study is composed of the following categories, (a) self-evaluation of 2D hand-drawn models, (b) verification of subparticulate levels, and (c) self-efficacy about students' performance.

### ***Self-Evaluation of 2D Hand-Drawn Models***

This category is defined as access to quickly check and generate 2D hand-drawn structures. Tools that provide students with feedback have shown increases in engagement and performance (Shea, 2016). MolView has a clean-up button that adjusts bond angles within the 2D virtual molecule. Students that were less confident in their 2D hand-drawn structures started their reaction mechanisms by entering the structure into MolView first, then copying the structure to paper; Jon expressed, "2D virtual model, it made it cleaner to look at." MolView enabled some students to start their practice to learn to content.

### ***Verification of Subparticulate Levels***

The definition of the category verification of subparticulate levels is using the 3D MolView representation for the subparticulate level to guide students through the reaction mechanism. Students indicated it was helpful at the start of the unit while they were still learning the reaction mechanism and why the reaction occurs. Bec stated, "I would [go to MolView if I was having a really rough time]" and Aston stated, "if I forgot

what was happening it would kind of remind me.” Sammie explained that it would have been helpful the year prior to understand subparticulate levels introduced in Chemistry 1: “it [MolView] adds an extra layer of like not a set of support [when learning about EN the first time in Chem 1], but kind of support just so you can fall back on.” Similar to the above category, this category is indicative of students’ engagement being affected by resources that provide feedback (Shea, 2016).

### ***Self-Efficacy About Students’ Performance***

Self-efficacy about students’ performance is defined as factors that influenced students’ perception to perform well in the context of chemical reaction mechanisms because of MolView. Most students communicated that MolView was interesting for various reasons, as stated by Sammie “3D, it's cool to see,” and Bec: “I thought it was really cool [3D rotation of molecules] because you can't do that on paper, so I thought it was really cool and I liked seeing stick out [3D virtual molecule].” This interest in virtual models created engagement with the content and helped support their motivation to learn the content even when there were minor issues or difficulties with the tool (Edwards et al., 2019; Lim et al., 2018). All students felt that they had improved and performed well in the post-assessment as indicated in the following statements:

Aston: the beginning of the unit, I was a little lost because. It was a little weird thinking about each step of the reaction...I definitely feel more confident [at the end of the unit].

Gracie: When I was writing this [open-ended short response questions], I feel like I knew exactly what to say.

Using MolView was easy enough for students to build upon existing schema as well as engaging. This ease and engagement helped build students self-efficacy in this unit.

### **Summary**

All students indicated finding various features of MolView as cool and interesting because they could see different properties of a molecule. This interest engaged students and motivated them to use the tool as a reference tool even after having developed conceptual understanding of the reaction mechanism. At the end of the four days of bellwork practice that instructed students to use MolView, no students were using MolView other than to check their own 2D hand-drawn structures. It seems that a good virtual tool may be intended for instructional purposes but over time should become a reference tool for students, if used at all.



## CHAPTER 5

### RESULTS

The purpose of this action research study was to assess how the use of three dimensional (3D) MolView virtual models influences high school students' ability to accurately understand and explain electron interactions in a chemical reaction after using the symbolic and subparticulate representational levels of understanding while attending a Chemistry 2 Honors course at Bellefield High School. A mixed method approach was used to collect data from interviews, articulation assessments, and a pre post-assessment. Data from these collection methods were used to answer the following research questions:

**RQ1:** How does students' ability to complete a reaction mechanism change after using 3D models to explore the symbolic and subparticulate representational levels of chemistry?

**RQ2:** How do students articulate the process of a reaction mechanism after manipulating 3D virtual models?

**RQ3:** What is the students' perception of using 3D models to learn a chemical reaction?

This chapter converges the prior studies and this study by presenting the (a) discussion, (b) implications, and (c) limitations.

#### Discussion

As a result of Johnstone's work in 1982 on delivering chemistry instruction built around the psychology of learning, quite controversial at the time, the Chemistry Triplet

was coined by Talanquer (2011). The triplet identifies three levels of understanding chemistry. One might consider each level as a perspective of thought defined by the type of information it encompasses. Each level of understanding and its information can be further characterized through representational models. This study demonstrates the usage of 3D dynamic virtual subparticulate level representations (see Figure 3.4) to explain the symbolic level around the framework of CLT. This mixed methods action research asks how students understanding is influenced by virtual representations of the subparticulate and symbolic levels in the context of an organic reaction mechanism. Qualitative and quantitative data was used collected to answer the research questions. Findings are situated within prior research and theories. This information is integrated below and organized by research question.

**Research Question 1: How does students' ability to complete a reaction mechanism change after using 3D models to explore the symbolic and subparticulate representational levels of chemistry?**

The subparticulate level was originally termed as explanatory by Johnstone (1982) to identify it as a means of communicating theory behind concepts represented symbolically. It is further defined as that which is inaccessible without imagination (Bucat & Mocerino, 2009). MolView was chosen because it allowed students to easily build molecules and select filters that make the inaccessible accessible to students (see Figure 3.4). The symbolic level communicates information through symbols (Johnstone, 2000; Gabel & Bunce, 1994) such as the familiar chemical formula or balanced equation (Gilbert & Treagust, 2009), as well as mathematical equations and reaction mechanisms (Kozma & Russell, 1997; Russel et al., 1997; Treagust et al., 2003) (see Figures 3.4). It is

defined as a means of communication information about the subparticulate level. Research by Bhattacharyya and Bodner (2005) and Gkitzia et al. (2019) indicates that students have difficulties moving between the symbolic and the subparticulate levels. Contrary to their work, students in this study were able to explain the symbolic and the subparticulate level. As indicated by Table 4.3, significant gains were made between the students' pre-post assessment which align with the quantitative results of the articulation assessment and excerpts from the assessment (see Appendix C). This is due to accounting for cognitive load and dual coding in the design of the instruction with MolView. The design of the instruction was effective because cognitive learning theory was used to organize the tasks within the lesson (Meissner & Bogner, 2013), and information processing was considered when determining how to activate prior knowledge in order to maximize working memory and schema theory. To start the unit, there was a whole group MolView orientation and guided practice of the reaction mechanism that had visual and auditory components. This corroborates Kirschner (2019) and Caviglioli (2019) findings indicating that making use of both auditory and visual systems maximizes the use of working memory and allows the information to move into long-term memory for recall later.

This study also reflects findings that dynamic representations can be useful for abstract concepts (Bodemer et al., 2004; Williamson & Abraham, 1995) but to a limit. MolView's 3D representations allowed students to add filters like the MEP lucent filter (see Figure 3.3) as well as manipulate the molecule with a touch pad or touch screen, which is defined as dynamic representation. Student responses in the interview align with findings that extraneous information from dynamic representations no longer aid learning

(Clark & Lyons, 2011; Jones, 2013; Jones et al., 2005; Suits, 2015; Suits & Sanger, 2013).

Students' interviews from this study align with Webber and Flynn's (2018) study finding a relationship between intrinsic motivation to self-correct explanations during an oral assessment and an increase in performance. While oral assessments were not used, participants shared that the discussions around the practice and usage of MolView supported conceptual development. Examples from interviews came from Gracie, "We got to see it through a different perspective, possibly just kind of opened our minds [through the whole group and small group discussions]," and Bec, "Especially like when you did it [MolView Group Act.] with partners, where we would have to explain with partners."

The articulation excerpts, interview, and pre-post assessment data indicates that students could apply both the subparticulate and symbolic level to a reaction mechanism with the implementation of MolView.

## **Research Question 2: How do students articulate the process of a reaction mechanism after manipulating 3D virtual models?**

Juggling multiple levels of understanding to fluently articulate chemical concepts requires "mental gymnastics" (Johnstone, 1982, p. 377). Virtual modeling, when appropriately selected and effectively applied to instruction, has been shown to improve students' understanding (Jones, 2013; Jones et al., 2005; Suits, 2015; Suits & Sanger, 2013) as indicated by the quantitative results of the articulation assessment of this study by maximizing working memory by making use of pre-existing schema (Driscoll, 2005) and minimizing cognitive load (Kirschner et al., 2018).

The risk of miscommunication between representations occurs when they are presented separately (Corradi et al., 2012) during instruction according to dual coding theory. Student interviews indicated the effectiveness of the MolView orientation activity as designed around schema theory and dual coding theory and due to familiarity with the prior representational models used in class (Good & Brophy, 1990) and from their own experience with representational models (Anderson, 2013). This concurs with Jung et al, (2022) whose work indicates the significance of schema theory for learning new and more complex information. For this portion of the lesson, students were all facing the Smartboard and were verbally guided to explain what they saw in a 3D virtual model. However, this first required activating prior knowledge. This study presented students with a color-coded world temperature map, similar to what they have seen in local weather forecasts or online weather mapping apps. This step was essential as it required students to recall weather forecast models and their use of color to represent temperature ranges and precipitation amounts. As a group, we discussed the idea of using colors to represent a concept and while students had this idea in their minds, they were then presented with a molecule in MolView with the 3D filter applied on the Smartboard. This step allowed students' working memory to be maximized as they were able to connect the new information to their pre-existing schema of colors representation models. It was at this time that students were then asked to think about properties of a molecule that could result in different colors on different parts of the molecule, further connecting the new content with content related pre-existing schema. They were then asked to discuss this with a student neighbor, and we then shared our ideas to confirm we all understood the notion of color representation in the new context. This active participation and attention

moved the from sensory memory to working memory. Participants made use developed schema weather maps to encode new information into long-term memory by modifying pre-existing content related schema to create mental images that were then used for retrieval during assessments and the interview (Driscoll, 2005).

Having begun the unit by connecting pre-existing schema to the new content, qualitative analysis of interviews, quantitative results of articulation and students' descriptions of their thought process during the articulation assessment indicate a strong ability to explain reaction mechanisms at the symbolic and subparticulate level. Quantitative results indicate they had the ability to store into and recall from long-term memory to develop and explanation that connected the subparticulate properties, as seen in MolView, to the symbolic representation of the reaction mechanism. Students used phrases like, "due to high/low electron dense regions," "due to formal charges." or "because of electronegativity..." when explaining their work on the post-assessment as opposed to concept-less statements like "this arrow moves here." In addition, statements were made indicating that they had developed and were using mental images to formulate their explanations, which students often do not make use of (Stull & Hegarty, 2016). Participants in this study were able to use more than one representational level of understanding because they were first reminded of models they have experience with, which were connected to the new 3D virtual model, followed by making further connections to prior domain specific knowledge to new content knowledge.

As in Bongers et al. (2020), Grove et al. (2012), Webber and Flynn (2018), and Flynn and Featherstone (2017), the qualitative and quantitative findings of this study

suggest that students' ability to articulate was influenced by the structure of the activities using MolView, unlike some participants in Gkitzia et al. (2019).

**Research Question 3: What is the students' perception of using 3D models to learn a chemical reaction?**

Qualitative data indicates that participants had a positive experience using MolView as they found it helpful in understanding subparticulate level concepts such as formal charge, electron density to make connections with the symbolic level of the reaction mechanism. Students in this study indicated that they liked using MolView up until a certain point, found it easy to use, that it was useful as a reference tool, and felt like it did help them understand the content.

Students found the introduction to the unit and the 3D representations helpful in both connecting the content to the representations and learning how to use MolView. Connecting it to prior knowledge and as an introduction to reaction mechanisms helped students see how the 3D representations were applied to the symbolic representation of a reaction mechanism (Anderson, 2013; Jung et al., 2022). As a class, we learned to read the 3D structures before introducing electron pushing formalism and the meaning of a reaction mechanism. We learned the subparticulate implications presented by the 3D structures, before applying the concepts to a more complicated 2D symbolic representation (Jung et al., 2022; Neumann & Kopcha, 2018). I believe this study clearly indicates students' ability to comprehend abstract topics because (a) virtual representations used were initially connected to their experiences and (b) the related pieces of the topic were introduced and discussed at the start. Once all participants

understood the smaller concepts, these concepts were applied to the content of Fischer Esterification reaction mechanisms.

All students used it to determine the relationship between electron density, electron pushing formalism, and the reaction mechanism. Students stated that because MolView had an interface that was easy to use and we had reviewed features together, they continued to use it but not as I had intended. This was mostly accomplished in the first two to three days of the innovation when they completed the Small Group MolView Activity and the first couple of sets of bellwork practice. After that, students indicated that while they liked MolView, they did not use it because they felt they had grasped the material. Participants indicated that while the bellwork instructions included using MolView, they did not once they were confident in their understanding. At this point, participants mostly referred back to MolView to check their 2D structures.

Student interviews also supported De Groot (1965) and Chase and Simon (1973) in that practice and seeing various examples helped students move information into long-term memory. All participants stated that it was because of MolView, the frequency of practice, the spaced practice, and MolView introduction that helped them put it all together. MolView never hindered their learning, but it was not MolView alone, supporting other studies warnings that the implementation of educational technology must be carefully planned (Al-Balushi & Coll, 2013; Antonoglou & Sigalas, 2011; Barrett et al., 2015; Stull et al., 2013).

Participants not only found MolView to be useful and cool, but they also liked seeing the molecules suggesting that using MolView increased engagement as seen in Edwards et al.'s (2019) virtual reality study. Similar to students in Shea's (2016) study,



which used Clickers for feedback, the qualitative analysis from student interviews indicated that these participants valued the feedback MolView could provide to assess their work. Shea's (2016) study noted an increase in teacher-student engagement due to the nature of their educational technology, qualitative and quantitative data showed that the engagement created by MolView and the resulting discussions around the feedback MolView provided supported students development of conceptual understanding.

The results of this study communicate what has been shared by Al-Balushi and Coll (2013), Antonoglou and Sigalas (2011), Barrett et al. (2015), and Stull et al. (2013), that chemical educational technology supports participants understanding with appropriate use. While participants in this study indicated that I requested they use MolView for too long, their interviews all clearly indicate that there were benefits to how MolView was used and that it was helpful in conceptualization as they could see the concepts being applied.

### **Implications**

Next, implications at three levels according to Kumar and Dawson (2014) will be presented, (a) personal implications, (b) implications for practice and immediate action, (c) implications for the future.

#### **Personal Implications**

There are many implications to my personal practice resulting from this study. Next, I will discuss my learning related to action research, interview and qualitative analysis and fulfilling my role as an educator.

### ***Action Research***

Most importantly, this study has been a reminder that important change can come from within (Mertler, 2020). Through this action research I have been able to find related work to further examine viable solutions to problems within my area of influence. It has been an impactful experience as it requires delving into research and theory to design a systematic means of collecting relevant data to assess the impact of an implemented plan. It has created an avenue for discussion not only with coworkers, but with students as well.

### ***Interview and Qualitative Analysis***

The interview and qualitative analysis process has left an imprint as it has been a reminder of the importance of the student perspective and evidence of Weinrich and Talanquer's (2016) caution that as teachers, we often neglect the developmental of student conceptualization. As time consuming as it was, it has proven an invaluable tool in my understanding of the student experience with instructional design. Without this component, I would not have identified the importance of components surrounding the usage of MolView. From this process I have been able to identify patterns, processes, and attitudes (Creswell, 2020) that I had not considered in the original design.

### ***Fulfilling My Role as an Instructor***

This study indicates that when designing instruction that uses representational models, virtual models should be used, if the model is selected and embedded within a lesson with great caution. Findings from this study have provided me with insight into how to better structure chemistry lessons around the application of multiple levels of understanding and check for understanding as assumptions and less efficient methods of

employment can lead to negative learning affects (Grosslight et al., 1991; Krell et al., 2014; Patron, 2017).

In doing so, this study demonstrates high school students' propensity to conceptually understand an organic reaction mechanism. Time must be taken to ensure students understand the basic features of the virtual model by activating prior knowledge and selecting models that are like previously used (and understood) by students. In addition, for this level content, participants benefited from (a) teacher-lead guided practice with the content and virtual model, and (b) ample and spaced practice with opportunities for discussion.

### **Implications For Practice and Immediate Action**

It is easy for instructors to assume that students grasp the salient features of a model and can apply it to the content (van Driel & Verloop, 1999). This may be because we, as chemistry instructors, are able to discern the intent behind models and assume the same understanding by students. It may also be due to our own lack of understanding of the purpose of the model (van Driel & Verloop, 1999). This study is a reminder of the importance for content area teachers to review educational technology, especially those intended to represent cause and effect or abstract concepts, together and explicitly discuss (a) the alignment of the tool and its features with learning objectives, (b) identify tool design functions and its virtual model features that could cause confusion for students, as well as (c) how to best roll out the tools implementation by making use of guided instruction and prior knowledge.

## **Future Implications**

Future studies should be constructed around the framework of constructivist and constructionism learning theories as a follow up to this lesson. From the interview portion, it was clear that discussions and interactions taking place around group work, using MolView and whole group practice were a crucial means of developing understanding for the participants in this study. This study did not have a novel reaction for participants to predict so how they process a novel reaction mechanism in a structured group activity could yield additional information as to (a) what features of a virtual representation students' focus on, (b) concepts are used to explain the mechanism, and (c) which thought processes are used to work through the mechanism. A second round of this study that included a novel reaction mechanism would further provide insight to students' ability to predict a reaction mechanism and how they construct their explanation. As chemistry education and state science standards reflect the NOS, action research studies like this will provide instructors insight as to how to best serve their students in the construction of lessons.

## **Limitations**

Action research by default has limitations to address due to the nature of action research, sample size and data collection instrument.

By nature, the design of action research limits generalization as its function is to find solutions to a local issue and resolve those issues in that context-specific area of influence (Creswell, 2017; Mertler, 2020). The results of this study cannot be generalized. The results of this study are specific to high-achieving second and third year high school chemistry students. Most studies related to organic chemistry are at the

college level with much larger sample sizes or middle school level with different chemistry content. The power dynamic existing between the student-teacher relationship must also be addressed. Students may have felt more pressure to communicate positively about their experience with MolView because I was in a higher position of authority (Mertler, 2020). Bias in interpretation of results should be addressed because I was both the researcher and instructor for the study (Mertler, 2020). To enhance the trustworthiness of this study, member checking, peer debriefing, and various instruments were used for data collection (Mertler, 2020). Throughout qualitative data collection, notes were recorded in a journal and continued to be made for self-reflexivity over the process. During analysis, participants were numbered instead of assigning names that I could associate with the original participant or from prior experiences. Once this paper was written, participant numbers were changed to pseudonyms for anonymity. Research notes, participant perspectives, and peer debriefing were all efforts to eliminate personal bias. In addition, the interview and articulation portion for this study were conducted over several weeks, increasing students' likelihood to inaccurately report their experience as time passed.

The small sample size for all components of the study is a limitation. This study was originally designed before COVID-19 and conducted two years later. Many students had switched to virtual educational programs which reduced in-person class sizes, temporarily. For the pre-post assessment  $n = 9$ , but for the interview and the articulation assessment,  $n = 6$ . A larger sample size approaching 20 participants would have yielded more data to strengthen the results (Creswell & Creswell, 2018) of this study.

Another limitation was the internal consistency reliability test for the prior-knowledge assessment. Kuder-Richardson 20 was below 0.70,  $\rho_{KR20} = 0.45$ , indicating that the items within the entry point knowledge check were not assessing the same underlying constructs as intended (Creswell & Creswell, 2018).

## REFERENCES

- Abel, R. R., & Kulhavy, R. W. (1989). Associating map features and related prose in memory. *Contemporary Educational Psychology*, 14(1), 33–48.
- Adeoye-Olatunde, O. A., & Olenik, N. L. (2021). Research and scholarly methods: Semi-structured interviews. *Journal of the American College of Clinical Pharmacy*, 4(10), 1358-1367.
- Ainsworth, S. (2008). The educational value of multiple-representations when learning complex scientific concepts. In J.K. Gilbert (Ed.), *Visualization: Theory and Practice in Science Education* (p. 191–208). Springer.
- Akerson, V. L., White, O., Colak, H., & Pongsanon, K. (2011). Relationships between elementary teachers' conceptions of scientific modeling and the nature of science. In *Models and Modeling*. Springer Netherlands. doi:10.1007/978-94-007-0449-7\_10
- Al-Balushi, S.M. (2009). Factors influencing pre-service science teachers' imagination at the microscopic level in chemistry. *International Journal of Science and Mathematics Education*, 7(6), 1089 – 1110.
- Al-Balushi, S. M., & Al-Hajri, S. H. (2014). Associating animations with concrete models to enhance students' comprehension of different visual representations in organic chemistry. *Chem. Educ. Res. Pract*, 15, 47. doi:10.1039/c3rp00074e
- Al-Balushi, S. M., & Coll, R. K. (2013). Exploring verbal, visual and schematic learners' static and dynamic mental images of scientific species and processes in relation to

- their spatial ability. *International Journal of Science Education*, 35(3), 460–489.  
doi:10.1080/09500693.2012.760210
- Aldahmash, A. H., & Abraham, M. R. (2009). Kinetic versus static visuals for facilitating college students' understanding of organic reaction mechanisms in chemistry. *Chemical Education Research*, 86(12), 1442–1446.
- Anderson, R. C. (2013). Role of the reader's schema in comprehension, learning, and memory. In D. E. Alvermann, N. Unrau & R. B. Ruddell (Eds.), *Theoretical Models and Processes of Reading* (p. 467–488). International Reading Association.
- Antonoglou, L., & Sigalas, M. P. (2011). Design, development and implementation of a technology enhanced hybrid course on molecular symmetry: Students' outcomes and attitudes. *Chemistry Education Research and Practice*, 12, 454–468.  
doi:10.1039/C0RP90013C
- Atkins, P. (2015). Foreword. In *Chemistry Education* (p. xxi–xxiv). Wiley.
- Atkinson, R. C., & Shiffrin, R. M. (1968). Human Memory: A Proposed System and Its Control Processes. In K. W. Spence, & J. T. Spence (Eds.), *The Psychology of Learning and Motivation: Advances in Research and Theory* (Vol. 2, pp. 89-195). Academic Press. doi.org/10.1016/s0079-7421(08)60422-3
- Austin, A. C., Ben-Daat, H., Zhu, M., Atkinson, R., Barrows, N., & Gould, I. R. (2015). Measuring student performance in general organic chemistry. *Chemistry Education Research and Practice*, 16(1), 168–178. doi:10.1039/c4rp00208c
- Baddeley, A. (2000). *The episodic buffer: A new component of working memory?*



- Barouillet, P., & Camos, V. (2007). The time-based resource-sharing model of working memory. In N. Osaka, R. H. Logie, & M. D'Esposito (Eds.), *The Cognitive Neuroscience of Working Memory* (p. 59–80). Oxford University Press.
- Barrett, T. J., Stull, A. T., Hsu, T. M., & Hegarty, M. (2015). Constrained interactivity for relating multiple representations in science: When virtual is better than real. *Computers and Education*, 81, 69–81. doi:10.1016/j.compedu.2014.09.009
- Bernard, H. R., Wutich, A., & Ryan, G. W. (2017). Q & A: Finding themes. In *Analyzing qualitative data: Systematic approaches* (2nd ed., p. 101–123). SAGE.  
doi:10.1145/2641223
- Bhattacharyya, G., & Bodner, G. M. (2014). Culturing reality: How organic chemistry graduate students develop into practitioners. *Journal of Research in Science Teaching*, 51(6), 694–713.
- Bhattacharyya, G., & Bodner, G. M. (2005). “It gets me to the product”: How students propose organic mechanisms. *Journal of Chemical Education*, 82(9), 1402–1407.  
doi:10.1021/ed082p1402
- Bloomberg, L., & Volpe, M. (2012). Presenting methodology and research approach. *Completing Your Qualitative Dissertation: A Roadmap from Beginning to End*, 65–93. doi:10.4135/9781452226613.n3
- Bodemer, D., Ploetzner, R., Feuerlein, I., & Spada, H. (2004). The active integration of information during learning with dynamic and interactive visualisations. *Learning and Instruction*, 14(3), 325–341. doi:10.1016/j.learninstruc.2004.06.006

- Bodner, G. M. (2015). Research on problem solving in chemistry. In J. Garcia-Martinez & E. Serrano-Torregrosa (Eds.), *Chem. Educ. Best Pract. Oppor. Trends* (p. 181-202). Wiley-VCH.
- Bongers, A., Beauvoir, B., Streja, N., Northoff, G., & Flynn, A. B. (2020). Building mental models of a reaction mechanism: the influence of static and animated representations, prior knowledge, and spatial ability. *Chemistry Education Research and Practice*. doi:10.1039/c9rp00198k
- Bongers, A., Northoff, G., & Flynn, A. B. (2019). Working with mental models to learn and visualize a new reaction mechanism. *Chemistry Education Research and Practice*, 20(3), 554–569. doi:10.1039/c9rp00060g
- Bowman, B. G., Karty, J. M., & Gooch, G. (2007). Teaching a modified Hendrickson, Cram, and Hammond Curriculum in organic chemistry. *Journal of Chemical Education*, 84(7). doi:10.1021/ed084p1209
- Brünken, R., Plass, J. L., & Leutner, D. (2003). Direct measurement of cognitive load in multimedia learning. *Educational Psychologist*, 38(1), 53–61.
- Bucat, R., & Mocerino, M. (2009). Learning at the sub-micro level: Structural representations. In J. K. Gilbert & D. Treagust (Eds.), *Multiple Representation in Chemical Education*. (p.11-29). Secaucus: Springer.
- Cai, S., Wang, X., & Chiang, F. K. (2014). A case study of augmented reality simulation system application in a chemistry course. *Computers in Human Behavior*, 37, 31–40. doi:10.1016/j.chb.2014.04.018
- Cambridge Dictionary. (2023). *conceptualize*. CambridgeWords. Retrieved from <https://dictionary.cambridge.org/us/dictionary/english/conceptualize>

- Cang, H., Shan Xu, C., & Yang, H. (2008). Progress in single-molecule tracking spectroscopy. *Chemical Physics Letters*, 457(4–6), 285–291.  
doi:10.1016/J.CPLETT.2008.03.098
- Caviglioli, O. (2019). *Dual Coding for Teachers*. John Catt Educational, Limited.
- Chandrasegaran, A. L., Treagust, D. F., & Mocerino, M. (2009). Emphasizing multiple levels of representation to enhance students' understandings of the changes occurring during chemical reactions. *Journal of Chemical Education*, 86(12), 1433–1436. doi:10.1021/ed086p1433
- Charmaz, K (2009). Example: The body, identity, and self: Adapting to impairment. In J.M. Morse, P. N. Stern, J. Corbin, B. Bowers, K. Charmaz, & A. E. Clarke, *Developing grounded theory: The second generation* (p. 155-91). Walnut Creek, Ca: Left Coast Press.
- Chen, O., Kalyuga, S., & Sweller, J. (2017). The expertise reversal effect is a variant of the more general element interactivity effect. *Educational Psychology Review*, 29(2). doi:10.1007/s10648-016-9359-1
- Cheng, M. M. W., & Gilbert, J. K. (2017). Modelling students' visualisation of chemical reaction. *International Journal of Science Education*, 39(9), 1173–1193.  
doi:10.1080/09500693.2017.1319989
- Chi, M. T. H. (1997). Quantifying qualitative analyses of verbal data: A Practical guide. *The Journal of The Learning Sciences*, 6(3), 271-315. Lawrence Erlbaum Associates, Inc.

- Childs, P. E., Markic, S., & Ryan, M. C. (2015). The role of language in the teaching and learning of chemistry. In J. Garcia-Martinez & E. Serrano-Torregrosa (Eds.), *Chemistry Education* (p. 421–446). Wiley.
- Chittleborough, G., & Treagust, D. F. (2007). The modeling ability of non-major Chemistry students and their understanding of the sub-microscopic level. *Chemistry Education Research and Practice*, 8(3), 274–292. doi: 10.1039/B6RP90035F
- Clark, R. C., & Lyons, C. (2011). *Graphics for learning: Proven guidelines for planning, designing, and evaluating visuals in training materials*. (2nd ed.). Pfeiffer.
- Clark, R. C., & Lyons, C. (2004). *Graphics for learning*. Wiley & Sons.
- Clough, M. P. (2006). Learners' responses to the demands of conceptual change: Considerations for effective nature of science instruction. *Science Education*, 15, 463–494. doi:10.1007/s11191-005-4846-7
- Corbin J., & Strauss, A. (2015) *Basics of qualitative research: Techniques and procedures for developing grounded theory* (4th ed.). Thousand Oaks, Ca: Sage.
- Corradi, D., Elen, J., & Clarebout, G. (2012). Understanding and enhancing the use of multiple external representations in chemistry education. *Journal of Science Education and Technology*, 21(6), 780–795. doi:10.1007/s10956-012-9366-z
- Cowan, N. (1995). *Attention and memory: An integrated framework*. Oxford University Press.
- Creswell, J. (2017). Data analysis and representation. In *Qualitative inquiry and research design: Choosing among the five traditions*. (p. 83–96). SAGE. doi:10.1201/9781351076418-7

- Creswell, J. W., & Plano Clark, V. L. (2006). *Designing and conducting mixed methods research*. SAGE. doi:10.1177/1049731508318695
- Creswell, J. W. (2014). *Research design: Qualitative, quantitative, and mixed methods approaches*. (4th ed., Issue 1). SAGE. doi:10.16309/j.cnki.issn.1007-1776.2003.03.004
- Creswell, J. W., & Creswell, J. D. (2018). *Research design: Qualitative, quantitative, and mixed methods approaches*. (5th ed.). SAGE.
- Czysz, K., Schroeder, L., & Clark, G. A. (2020). Making acids and bases more basic: Supporting students' conceptualization of acid-base chemistry through a laboratory exercise that connects molecular-level representations to symbolic representations and experimentally derived evidence. *Journal of Chemical Education*, 97(2), 484–489. doi:10.1021/acs.jchemed.9b00645
- Deng, F., Chen, D.T., Tsai, C.C., & Chai, C. S. (2011). Students' views of the nature of science: A critical review of research. *Science Education*, 95(6), 961–999. doi:10.1002/SCE.20460
- Denscombe, M. (2008). Communities of practice. A research paradigm for the mixed methods approach. *Journal of Mixed Methods Research*, 2(3), 270–283.
- Driscoll, M. P. (2005). Cognitive information processing. In *Psychology of Learning for Instruction* (3rd ed., p. 71–110). Pearson.
- Dzurec, L. C., & Abraham, J. L. (1993). The nature of inquiry: Linking quantitative and qualitative research. *Advances in Nursing Science*, 16, 73–79.
- Ericsson, K. A., & Simon, H. A. (1993). *Protocol analysis: Verbal reports as data*. MIT Press.

- Edwards, B. I., Bielawski, K. S., Prada, R., & Cheok, A. D. (2019). Haptic virtual reality and immersive learning for enhanced organic chemistry instruction. *Virtual Reality, 23*(4), 363–373. doi:10.1007/s10055-018-0345-4
- Fetters, M. D., Curry, L. A., & Creswell, J. W. (2013). Achieving integration in mixed methods designs - Principles and practices. *Health Services Research, 48*(6 PART2), 2134–2156. doi:10.1111/1475-6773.12117
- Fiorella, L., & Zhang, Q. (2018). Drawing boundary conditions for learning by drawing. In *Educational Psychology Review, 30*(3), 1115–1137.
- Fjeld, M., Juchli, P., Fredriksson, J., Ejdestig, M., Duca, F., Bötschi, K., & Voegtli, B. (2007). Tangible user interface for chemistry education: Comparative Evaluation and Re-Design. *CHI '07: Proceedings of the SIGCHI Conference on Human Factors in Computing Systems*, 805–808. doi:10.1145/1240624.1240745
- Fleming, M. (1987). Displays and communication. In R. Gagné (Ed.), *Instructional technology foundations* (p. 233–260). Lawrence Erlbaum Associates.
- Flynn, A. B., & Featherstone, R. B. (2017). Language of mechanisms: Exam analysis reveals students' strengths, strategies, and errors when using the electron-pushing formalism (curved arrows) in new reactions. *Chemistry Education Research and Practice, 18*(1), 64–77. doi:10.1039/c6rp00126b
- Gabel, D. L. (1998). The complexity of chemistry and its implications for teaching. In *International handbook of science education* (p. 223–248). Kluwer.
- Gabel, D. L. (1999). Improving teaching and learning through chemistry education research: A look to the future. *Journal of Chemical Education, 76*(4).  
<https://pubs.acs.org/sharingguidelines>

- Gabel, D. L. (1993). Use of the particle nature of matter in developing conceptual understanding. *Journal of Chemical Education*, 70(3), 193–194.  
<https://pubs.acs.org/sharingguidelines>
- Gabel, D. L., & Bunce, D. M. (1994). Handbook of research on science teaching and learning. *Handbook of Research on Science Teaching and Learning*, 11, 301–326.
- Galloway, K. R., Stoyanovich, C., & Flynn, A. B. (2017). Students' interpretations of mechanistic language in organic chemistry before learning reactions. *Chemistry Education Research and Practice*, 18(2), 353–374. doi:10.1039/c6rp00231e
- Gilbert, J. K., Boulter, C. J., & Elmer, R. (2000). Positioning models in science education and in design and technology education. In J. K. Gilbert & C. J. Boulter (Eds.), *Developing Models in Science Education* (p. 3–18). Dordrecht: Kluwer.
- Gilbert J. K., & Treagust, D. (2009). Introduction: Macro, submicro and symbolic representations and the relationship between them: Key models in chemical education. In J. K. Gilbert & D. Treagust (Eds.), *Multiple Representations in Chemistry Education* (p. 1–10). Springer. doi:10.1007/978-1-4020-8872-8
- Gilbert, J. K., & Afonso, A. S. (2015). Lifelong learning: Approaches to increasing the understanding of chemistry by everybody. In J. Garcia-Martinez & E. Serrano-Torregrosa (Eds.), *Chemistry Education*: (p. 123–148). Wiley-VCH.
- Gkitzia, V., Salta, K., & Tzougraki, C. (2019). Students' competence in translating between different types of chemical representations. *Chemistry Education Research and Practice*. doi:10.1039/c8rp00301g
- Glaser, B. G., & Stauss, A. L. (1967). *The discovery of grounded theory*. Aldine de Gruyter.

- Glesne, C. (2006). *Becoming qualitative researchers: An introduction* (3rd ed.). Longman.
- Grosslight, L., Unger, C., Jay, E., & Smith, C. L. (1991). Understanding models and their use in science: Conceptions of middle and high school students and experts. *Journal of Research in Science Teaching*, 28(9). doi:10.1002/tea.3660280907
- Grove, N. P., Cooper, M. M., & Cox, E. L. (2012). Does mechanistic thinking improve student success in organic chemistry? *Journal of Chemical Education*, 89(7), 850–853. doi:10.1021/ed200394d
- Grünkorn, J., Upmeier Zu Belzen, A., & Krüger, D. (2014). Assessing students' understandings of biological models and their use in science to evaluate a theoretical framework. *International Journal of Science Education*, 36(10), 1651–1684. doi:10.1080/09500693.2013.873155
- Hamilton, A. B., & Finley, E. P. (2019). Qualitative methods in implementation research: An introduction. *Psychiatry Research*, 280. doi:10.1016/j.psychres.2019.112516
- Hannafin, M. J., & Rieber, L. P. (1989). Psychological foundations of instructional design for emerging computer-based instructional technologies: Part I. *Educational Technology Research and Development*, 37(2), 91–101.
- Hanson, W. E., Plano Clark, V. L., Petska, K. S., Creswell, J. W., & Creswell, J. D. (2005). Mixed methods research designs in counseling psychology. *Journal of Counseling Psychology*, 52(2), 224–235. doi:10.1037/0022-0167.52.2.224
- Harris, P. A. (2019). *Spatializing an undergraduate chemistry curriculum: Action research to assist students with low visual-spatial ability* (Issue February).



- Harrison, A. G., & Treagust, D. F. (1996). Secondary students' mental models of atoms and molecules: Implications for teaching chemistry. *Science Education*, 80(5).  
[https://doi.org/10.1002/\(SICI\)1098-237X\(199609\)80:5<509::AID-SCE2>3.0.CO;2-F](https://doi.org/10.1002/(SICI)1098-237X(199609)80:5<509::AID-SCE2>3.0.CO;2-F)
- Herr, K., & Anderson, G. (2005). The continuum of positionality in action research. In *The action research dissertation: A guide for students and faculty* (p. 29–42). SAGE Publications, Inc. doi:10.4135/9781452226644
- Howe, C. (2014). Optimizing small group discourse in classrooms: Effective practices and theoretical constraints. *International Journal of Education*, 63, 107–115.  
 doi:10.1016/j.ijer.2013.03.011
- Jaber, L. Z., & BouJaoude, S. (2012). A macro-micro-symbolic teaching to promote relational understanding of chemical reactions. *International Journal of Science Education*, 34(7), 973–998. doi:10.1080/09500693.2011.569959
- Jick, T. D. (1979). Mixing qualitative and quantitative methods: Triangulation in action. *Administrative Science Quarterly*, 24(4), 602–611. doi:10.2307/2392366
- Johnstone, A. H. (1982). Macro and microchemistry. *School Science Review*, 64, 377–379.
- Johnstone, A. H. (1989). Some messages for teachers and examiners: An information processing model. In *Assessment of Chemistry in Schools* (Vol. 7, p. 23–39). Royal Society of Chemistry Education Division.
- Johnstone, A. H. (1991). Why is science difficult to learn? Things are seldom what they seem. *Journal of Computer Assisted Learning*, 7(2). doi:10.1111/j.1365-2729.1991.tb00230.x

- Johnstone, A. H. (1993). The development of chemistry teaching: A changing response to changing demand. *Journal of Chemical Education*, 70(9), 701–705. doi: 10.1021/ed070p701
- Johnstone, A. H. (2000). Teaching of chemistry: Logical or psychological? *Chem. Educ. Res. Pract.*, 1(1), 9–15. doi:10.1039/a9rp90001b
- Jones, L. L. (2013). *How Multimedia-Based Learning and Molecular Visualization Change the Landscape of Chemical Education Research*. doi:10.1021/ed4001206
- Jones, L. L., Jordan, K. D., & Stillings, N. A. (2005). Molecular visualization in chemistry education: the role of multidisciplinary collaboration. In *Chemistry Education Research and Practice* (Vol. 6, Issue 3, p. 136–149).
- Jonsen, K., & Jehn, K. A. (2009). Using triangulation to validate themes in qualitative studies. *Qualitative Research in Organizations and Management*, 4(2), 135–150. doi:10.1108/17465640910978391
- Jung E, Lim R, Kim D. (2022). A Schema-Based Instructional Design Model for Self-Paced Learning Environments. *Education Sciences*, 12(4), 271. [doi.org/10.3390/educsci12040271](https://doi.org/10.3390/educsci12040271)
- Kelly, R. M., Akaygun, S., Hansen, S. J. R., & Villalta-Cerdas, A. (2017). The effect that comparing molecular animations of varying accuracy has on students' submicroscopic explanations. *Chemistry Education Research and Practice*, 18(4), 582–600. doi:10.1039/c6rp00240d
- Keiner, L., & Graulich, N. (2019). Transitions between representational levels: Characterization of organic chemistry students' laboratory work-up procedures. *Chemistry Education Research and Practice*. doi:10.1039/c9rp00241c

- Kermack, W. O., & Robinson, R. (1922). An explanation of the property of induced polarity of atoms and an interpretation of the theory of partial valencies on an electronic basis. *Journal of the Chemical Society, Transactions*, 121, 427–440. doi:10.1039/CT9222100427
- Kim, S. Y., & Irving, K. E. (2009). History of science as an instructional context: Student learning in genetics and nature of science. *Science & Education* 2009 19:2, 19(2), 187–215. doi:10.1007/S11191-009-9191-9
- Kirschner, P. A., Sweller, J., Kirschner, F., & Zambrano, J. R. (2018). From cognitive load theory to collaborative cognitive load theory. *International Journal of Computer-Supported Collaborative Learning*, 13(2), 213–233. doi:10.1007/s11412-018-9277-y
- Klahr, D., Triona, L. M., & Williams, C. (2007). Hands on what? The relative effectiveness of physical versus virtual materials in an engineering design project by middle school children. *Journal of Research in Science Teaching*, 44(1), 183–203.
- Kozma, R. (2003). The material features of multiple representations and their cognitive and social affordances for science understanding. *Learning and Instruction*, 13(2), 205–226. doi:10.1016/s0959-4752(02)00021-x
- Kozma, R. B., & Russell, J. (1997). Multimedia and understanding: Expert and novice responses to different representations of chemical phenomena. *Journal of Research in Science Teaching*, 34(9), 949–968.

- Krell, M., Upmeier zu Belzen, A., & Krüger, D. (2014). Students' levels of understanding models and modeling in biology: Global or aspect-dependent? *Research in Science Education*, 44(1), 109–132. doi:10.1007/s11165-013-9365-y
- Kulhavy, R. W., Stock, W. A., & Kealy, W. A. (1993). How geographic maps increase recall of instructional text. *Educational Technology Research and Development*, 41(4), 47–62.
- Lederman, N. G. (2007). Nature of science: Past, present, and future. In S. K. Abell & N. G. Lederman (Eds.), *Handbook of Research on Science Education* (p. 831–879). Lawrence Erlbaum Associates.
- Lim, K. Y. T., Chen, K. H.C., Lin, S.W., Huang, J.C., Ng, K. S.E., Ng, J. J. L., Wang, Y., & Woong, N. (2018). Representations of novice conceptions with learner-generated augmentation: A framework for curriculum design with augmented reality. *Journal For Virtual Worlds Research*, 11(3), 1–20.  
doi:10.4101/jvwr.v11i3.7327
- Lin, Y. I., Son, J. Y., & Rudd, J. A. (2016). Asymmetric translation between multiple representations in chemistry. *International Journal of Science Education*, 38(4), 644–662. doi:10.1080/09500693.2016.1144945
- Lowe, D. G. (2004). Distinctive image features from scale-invariant keypoints. *International Journal of Computer Vision*, 60, 91–110.
- Mahaffy, P. (2015). Chemistry education and human activity. In J. Garcia-Martinez & E. Serrano-Torregrosa (Eds.), *Chem. Educ. Best Pract. Oppor. Trends* (p. 3-26). Wiley-VCH.

- Martinez-Jimenez, P., Pontes-Pedrajas, A., Polo, J., & Climent-Bellido, M. S. (2003). Learning in chemistry with virtual laboratories. *Journal of Chemical Education*, 80(3), 346–352. <http://www.uco.es/grupos/>
- Mayer, R. E. (2009). *Multimedia learning* (2nd ed.). Cambridge University Press.
- Mayer, R. E. (2014). Handbook of Research on Educational Communications and Technology. In J. M. Spector, M. D. Merrill, J. Elen, & M. J. Bishop (Eds.), *Handbook of Research on Educational Communications and Technology: Fourth Edition* (4th ed.). Springer. doi:10.1007/978-1-4614-3185-5
- Mayer, R. E., Hegarty, M., Mayer, S., & Campbell, J. (2005). When static media promote active learning: Annotated illustrations versus narrated animations in multimedia instruction. *Journal of Experimental Psychology: Applied*, 11(4), 256–265. doi:10.1037/1076-898X.11.4.256
- Meissner, B., & Bogner, F. X. (2013). Towards cognitive load theory as guideline for instructional design in science education. *World Journal of Education*, 3(2). doi:10.5430/wje.v3n2p24
- Merriam, S. B., & Tisdell, E. J. (2015). Qualitative data analysis. In *Qualitative research: A guide to design and implementation* (p. 195–236). John Wiley & Sons, Incorporated.
- Merriam-Webster. (n.d.). *Three-dimensional*. Merriam-Webster.Com Dictionary. Retrieved May 28, 2021, from <https://www.merriam-webster.com/dictionary/three-dimensional>

- Merriam-Webster. (n.d.). *Two-dimensional*. Merriam-Webster.Com Dictionary.  
Retrieved May 28, 2021, from <https://www.merriam-webster.com/dictionary/two-dimensional>
- Mertler, C. A. (2020). *Action research: Improving schools and empowering educators* (6th ed.). SAGE.
- Miller, G. A. (1956). The magic number seven, plus or minus two: Some limits to our capacity for processing information. *Psychological Review*, 63, 81–97.
- Moyer, P. S., Bolyard, J. J., & Spikell, M. A. (2002). What are virtual manipulatives? *Teaching Children Mathematics*, 8, 372–377.
- Nahum, T. L., Hofstein, A., Mamlock-Naaman, R., & Bar-Dov, Z. (2004). Can final examinations amplify students' misconceptions in chemistry? *Chem. Educ. Res. Pract.*, 5(3). doi:10.1039/B4RP90029D
- Nakhleh, M. B., & Krajcik, J. S. (1994). Influence of level of information as presented by different technologies on students' understanding of acid, base and pH concepts. *Journal of Research in Science Teaching*, 31(10), 1077–1096.
- Nakhleh, M. B. (1992). Why some students don't learn chemistry: Chemical misconceptions. *Journal of Chemical Education*, 191–196.
- National Academy of Sciences. (2013). *Appendix H- Understanding the scientific enterprise: The nature of science in the next generation science standards. A framework for K-12 science education*.
- National Research Council. (1996). *National science education standards: Observe, interact, change, learn*. National Academy Press.

- National Research Council. (2007). *Taking science to school: Learning and teaching science in grades K-8*. National Academies Press.
- National Research Council. (2012). *A Framework for K-12 Science Education: Practices, Crosscutting Concepts*. National Academic Press.
- Neumann, K. L., & Kopcha, T. J. (2018). The Use of Schema Theory in Learning, Design, and Technology. *Tech Trends*, 62(5), 429–431. [doi.org/10.1007/s11528-018-0319-0](https://doi.org/10.1007/s11528-018-0319-0)
- Oh, P. S., & Oh, S. J. (2011). What teachers of science need to know about models: An overview. *International Journal of Science Education*, 33(8), 1109–1130.  
doi:10.1080/09500693.2010.502191
- Owen, W. F. (1984). Interpretive themes in relational communication. *Quarterly Journal of Speech*, 70(3).
- Paas, F., Renkl, A., & Sweller, J. (2003). Cognitive load theory and instructional design: recent developments. *Educational Psychologist*, 38(1).
- Parsons, R. D., & Brown, K. S. (2002). *Teacher as reflective practitioner and action researcher*. Wadsworth/Thomson Learning.
- Patron, E., Wikman, S., Edfors, I., Johansson-Cederblad, B., & Linder, C. (2017). Teachers' reasoning: Classroom visual representational practices in the context of introductory chemical bonding. *Science Education*, 101(6), 887–906.  
doi:10.1002/sce.21298
- Pearce, E. (2002). Reinventing chemical education. *Chemical and Engineering News*.

- Penn, J. H., & Al-Shammari, A. G. (2008). Teaching reaction mechanisms using the curved arrow neglect (CAN) method. *Journal of Chemical Education*, 85(9), 1291–1295.
- Permana, I., Firman, H., Redjeki, S., & Hamidah, I. (2019). Applying of teaching strategy based on cognitive load theory to develop pre-service teacher teaching skills of waves: Cognitive load analysis. *Journal of Physics: Conference Series*, 1157(2), 1–8. doi:10.1088/1742-6596/1157/2/022026
- Poincaré, H. (1952). *Science and hypothesis* (New Dover ed. unabridged republ. of the first english transl). Dover Publ.
- Punch, K. (2014). *Introduction to social research* (3<sup>rd</sup> ed.). London, UK: SAGE.
- Rankin, R. O. (1989). The development of an illustration design model. *Educational Technology Research and Development*, 37(2). doi:10.1007/BF02298288
- Rau, M. A. (2018). Making connections among multiple visual representations: how do sense-making skills and perceptual fluency relate to learning of chemistry knowledge? *Instructional Science*, 46(2), 209–243. doi:10.1007/s11251-017-9431-3
- Rogers, J. R. (2012). *Modification of instructional delivery and student learning with the use of educational technologies*. 3548868
- Rop, G., van Wermeskerken, M., de Nooijer, J. A., Verkoeijen, P. P. J. L., & van Gog, T. (2018). Task experience as a boundary condition for the negative effects of irrelevant information on learning. *Educational Psychology Review*, 30(1), 229–253. doi:10.1007/s10648-016-9388-9



- Rossmann, G. B., & Wilson, B. L. (1985). Numbers and words: Combining quantitative and qualitative methods in a single large-scale evaluation study. *Evaluation Review*, 9, 627–643.
- Rowe, M. B. (1983). Getting chemistry off the killer course list. *Journal of Chemical Education*, 60(11), 954. doi:10.1021/ed060p954
- Rubin H. J. & Rubin I. (2011). *Qualitative interviewing: the art of hearing data* (3<sup>rd</sup> Ed.). SAGE.
- Rumelhart, D. E., & Norman, D. A. (1978). Accretion, tuning, and restructuring: Three modes of learning. In J. W. Cotton & R. L. Klatzky (Eds.), *Semantic Factors in Cognition* (p. 37–53). Lawrence Erlbaum Associates.
- Russell, J. W., Kozma, R. B., Jones, T., Wykoff, J., Marx, N., & Davis, J. (1997). Use of simultaneous-synchronized macroscopic, microscopic, and symbolic representations to enhance the teaching and learning of chemical concepts. *Journal of Chemical Education*, 74(3), 330–334. doi:10.1021/ed074p330
- Saldaña, J. (2009). An introduction to codes and coding. In *The coding manual for qualitative researchers*. SAGE. doi:10.1002/9780470975220.ch1
- Saldaña, J. (2016). *The coding manual for qualitative researchers*. SAGE.
- Sandelowski, M., Voils, C. I., & Knafl, G. (2009). On quantizing. *Journal of Mixed Methods Research*, 3(3), 208–222.
- Schmuck, R. A. (1997). *Practical action research for change*. SkyLight Professional Development.

- Schnotz, W. (2005). An integrated model of text and picture comprehension. In R.E. Mayer (Ed.), *The Cambridge handbook of multimedia learning* (p. 49–69). Cambridge University Press.
- Schwalbach, E. M. (2003). *Value and validity in action research: A guidebook for reflective practitioners*. Lanham, MD: Scarecrow Press.
- Schwarz, C. V., Reiser, B. J., Davis, E. A., Kenyon, L., Achér, A., Fortus, D., Shwartz, Y., Hug, B., & Krajcik, J. (2009). Developing a learning progression for scientific modeling: Making scientific modeling accessible and meaningful for learners. *Journal of Research in Science Teaching*, 46(6), 632–654. doi:10.1002/tea.20311
- Sechrest, L., & Sidana, S. (1995). Quantitative and qualitative methods: Is there an alternative? *Evaluation and Program Planning*, 18, 77–87.
- Sen, A., Mai, T., Kastberg, D., Cummings, L., & Perkins, R. (2019). Highlights of U.S. PISA 2018 Results Web Report. *National Center for Educational Statistics*, 1–64. <https://nces.ed.gov/pubsearch/pubsinfo.asp?pubid=2020166>
- Seufert, T. (2003). Supporting coherence formation in learning from multiple representations. *Learn Instr*, 13, 227–233.
- Shea, K. M. (2016). Beyond clickers, next generation classroom response systems for organic chemistry. *Journal of Chemical Education*, 93(5), 971–974. doi:10.1021/acs.jchemed.5b00799
- Shenton, A. K. (2004). Strategies for ensuring trustworthiness in qualitative research projects. *Education For Information*, 22(3), 63–75.

- Shwartz, Y., Ben-Zvi, R., & Hofstein, A. (2006). The use of scientific literacy taxonomy for assessing the development of chemical literacy among high-school students. *Chemical Education Research and Practice*, 7(4), 203–225.
- Soderqvist, T. (Ed.). (1997). *The Historiography of Contemporary Science and Technology*. Harwood Academic Publishers.
- Songer, N. B., & Linn, M. C. (1991). How do students' views of science influence knowledge integration? *Journal of Research in Science Teaching*, 28(9), 761–784.
- Starbek, P., Starčič Erjavec, M., & Peklaj, C. (2010). Teaching genetics with multimedia results in better acquisition of knowledge and improvement in comprehension. *Journal of Computer Assisted Learning*, 26(3), 214–224.
- Stieff, M., Bateman, R., & Uttal, D. H. (2005). Teaching and learning with three-dimensional representations. In J.K. Gilbert (Ed.), *Visualization in Science Education* (p. 93–118). Springer. doi:10.1007/1-4020-3613-2\_7
- Stieff, M., Hegarty, M., & Deslongchamps, G. (2011). Identifying representational competence with multi-representational displays. *Cognition and Instruction*, 29(1), 123–145. doi:10.1080/07370008.2010.507318
- Stieff, M., Scopelitis, S., Lira, M. E., & Desutter, D. (2016). Improving representational competence with concrete models. *Science Education*, 100(2), 344–363. doi:10.1002/sce.21203
- Strauss, A. L. (1987). *Qualitative analysis for social scientists*. Cambridge University Press.

- Stull, A. T., Barrett, T., & Hegarty, M. (2013). Usability of concrete and virtual models in chemistry instruction. *Computers in Human Behavior*, 29(6), 2546–2556. doi:10.1016/j.chb.2013.06.012
- Stull, A. T., Gainer, M., Padalkar, S., & Hegarty, M. (2016). Promoting representational competence with molecular models in organic chemistry. *Journal of Chemical Education*, 93(6), 994–1001. doi:10.1021/acs.jchemed.6b00194
- Stull, A. T., & Hegarty, M. (2016). Model manipulation and learning: Fostering representational competence with virtual and concrete models. *Journal of Educational Psychology*, 108(4), 509–527. doi:10.1037/edu0000077
- Suits J. P. (2015). Design of dynamic visualizations to enhance conceptual understanding in chemistry courses. In J. Garcia-Martinez & E. Serrano-Torregrosa (Eds.), *Chem. Educ. Best Pract. Oppor. Trends* (p. 595–619). Wiley-VCH.
- Suits, J. P., & Sanger, M. J. (2013). Dynamic visualizations in chemistry courses. *ACS Symposium Series*, 1142(c), 1–13. doi:10.1021/bk-2013-1142.ch001
- Sweller, J., Ayres, P., & Kalyuga, S. (2011). *Cognitive load theory: Explorations in the learning sciences, instructional systems and performance technologies*. Springer. doi:10.1007/978-1-4419-8126-4\_2
- Sweller, J.; Van Merriënboer, J.J.G.; Paas, F. (1998). Cognitive Architecture and Instructional Design. *Educ. Psychol. Rev.* 10, 251–296.
- Sweller, J. (2020). Cognitive load theory and educational technology. *Educational Technology Research and Development*, 68(1), 1–16. doi:10.1007/s11423-019-09701-3

- Taber, K. S. (2002). *Chemical misconceptions: Prevention, diagnosis and cure. Vol. 1: Theoretical Background*. (Vol. 1). Royal Society of Chemistry.
- Taber, K. S. (2013). Revisiting the chemistry triplet: Drawing upon the nature of chemical knowledge and the psychology of learning to inform chemistry education. *Chemistry Education Research and Practice*, 14(2), 156–168.  
doi:10.1039/c3rp00012e
- Taber, K. S. (2014). The significance of implicit knowledge for learning and teaching chemistry. *Chemistry Education Research and Practice*, 15(4), 447–461.  
doi:10.1039/c4rp00124a
- Taber, K. S. (2015). The role of conceptual integration in understanding and learning chemistry. In J. Garcia-Martinez & E. Serrano-Torregrosa (Eds.), *Chemistry Education: Best Practices, Opportunities and Trends* (p. 375–394). Wiley-VCH.
- Talanquer, V. (2007). Explanations and teleology in chemistry education. *International Journal of Science Education*, 29(7), 853–870. doi:10.1080/09500690601087632
- Talanquer, V. (2011). Macro, submicro, and symbolic: The many faces of the chemistry “triplet.” *International Journal of Science Education*, 33(2), 179–195.  
doi:10.1080/09500690903386435
- Tasker, R., & Dalton, R. (2008). Visualizing the molecular world: Design, evaluation, and use of animations. In *Visualization: Theory and Practice in Science Education*, 3.
- Teye, A. C., & Peaslee, L. (2015). Measuring educational outcomes for at-risk children and youth: Issues with the validity of self-reported data. *Child and Youth Care Forum*, 44(6), 853–873. doi:10.1007/s10566-015-9310-5

- Tracy, S. J. (2020). *Qualitative research methods: Collecting evidence, crafting analysis, communicating impact* (2nd Ed.). Wiley.
- Treagust, D. F., & Chittleborough, G. (2001). Chemistry: A matter of understanding representations. In J. Brophy (Ed.), *Subject-Specific Instructional Methods and Activities* (p. 239–267). Elsevier.
- Treagust, D. F., Chittleborough, G., & Mamiala, T. L. (2003). The role of submicroscopic and symbolic representations in chemical explanations. *International Journal of Science Education*, 25(11), 1353–1368. doi:10.1080/0950069032000070306
- U.S. Department of Education. (2020). Science, technology, engineering, and math, including computer science. In *U.S. Department of Education*.  
<https://www.ed.gov/stem>
- U.S. Department of Education. Institute of Education Sciences, N. C. for E. S. (2020). Highlights of U.S. PISA 2018 Results Web Report. In *U.S. Department of Education. Institute of Education Sciences, National Center for Education Statistics*. <https://nces.ed.gov/surveys/pisa/pisa2018/index.asp.%0A%0A>
- van Driel, J. H., & Verloop, N. (1999). Developing science teachers' knowledge on models and modeling. *International Journal of Science Education*, 21(11), 1141–1153. doi:10.1007/1-4020-3699-X\_10
- van Lanen, R. J., McGannon, T., & Lockie, N. M. (2000). Predictors of nursing students' performance in a one-semester organic and biochemistry course. *Journal of Chemical Education*, 77(6), 767. doi:10.1021/ed077p767
- van Someren, M. W., Barnard, Y. F., & Sandberg, J. A. C. (1994). *The think-aloud method: A practical guide to modeling cognitive processes*. Academic Press

- Vogt, W. P., Vogt, E. R., Gardner, D. C., & Haeffke, L. M. (2014). *Selecting the right analysis for your data: Quantitative, qualitative, and mixed methods*. Guilford.
- Wang, C. Y., & Barrow, L. H. (2011). Characteristics and levels of sophistication: An analysis of chemistry students' ability to think with mental models. *Research in Science Education*, 41(4), 561–586. doi:10.1007/s11165-010-9180-7
- Webber, D. M., & Flynn, A. B. (2018). How are students solving familiar and unfamiliar organic chemistry mechanism questions in a new curriculum? *Journal of Chemical Education*, 95(9), 1451–1467. doi:10.1021/acs.jchemed.8b00158
- Weeks, D. P. (1967). Successful student seminars. *Journal of Chemical Education*, 44, 290–294.
- Weinrich, M. L., & Talanquer, V. (2016). Mapping students' modes of reasoning when thinking about chemical reactions used to make a desired product. *Chemistry Education Research and Practice*, 17(2), 394–406. doi:10.1039/c5rp00208g
- Wentland, S. H. (1994). A new approach to teaching organic chemical mechanisms. *J. Chem. Educ.*, 71(1), 3–8.
- West, C. K., Farmer, J. A., & Wolff, P. M. (1991). Introduction to cognitive science and instructional design. *Instructional Design Implications from Cognitive Science* (p. 1–35). Prentice Hall.
- Williams, G., & Clement, J. (2015). Identifying multiple levels of discussion-based teaching strategies for constructing scientific models. *International Journal of Science Education*, 37(1), 82–107. doi:10.1080/09500693.2014.966257

- Williamson, V. M., & Abraham, M. R. (1995). The effects of computer animation on the particulate mental models of college chemistry students. *Journal of Research in Science Teaching*, 32(5), 521–534.
- Winn, W. (1989). The design and use of instructional graphics. In H. Mandl & J. R. Levin (Eds.), *Advances in Psychology* (Vol. 58, p.125–144). Elsevier Science Publishers.
- Winn, W. (2004). Cognitive perspectives in psychology. In D. H. Jonassen (Ed.), *Handbook of Research on Educational Communications and Technology* (2nd ed., p. 79–112). Lawrence Erlbaum Associates.
- Yang, C., Jen, C. H., Chang, C. Y., & Yeh, T. K. (2018). Comparison of animation and static-picture based instruction: Effects on performance and cognitive load for learning genetics. *Educational Technology and Society*, 21(4), 1-11.
- Ye, J., Lu, S., & Bi, H. (2018). The effects of microcomputer- based laboratories on students macro, micro, and symbolic representations when learning about net ionic reactions. *Chemistry Education Research and Practice*, 20, 288–301.  
doi:10.1039/C8RP00165K
- Zacharia, Z. C., & Olympiou, G. (2011). Physical versus virtual manipulative experimentation in physics learning. *Learning and Instruction*, 21, 317–331.



APPENDIX A

PRE- AND POST-TEST

Name: \_\_\_\_\_ Block: \_\_\_\_\_ Date: \_\_\_\_\_

Select the best answer for the multiple-choice questions.

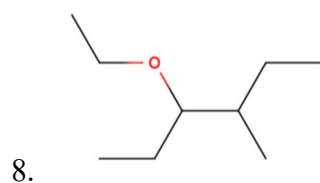
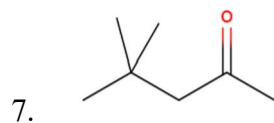
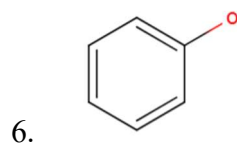
1. Which element of the set has a higher electronegativity value?
  - a. Ca
  - b. Br
  - c. S
  - d. Zn
  - e. I am not sure
  
2. Which of the set has a lower electronegativity value?
  - a. Ca
  - b. Br
  - c. S
  - d. Zn
  - e. I am not sure
  
3. Draw a molecule with four carbons containing a carboxyl group. Circle the carboxyl group in your work.

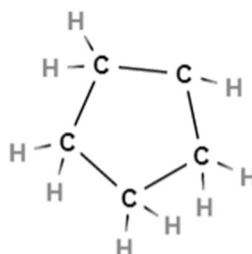
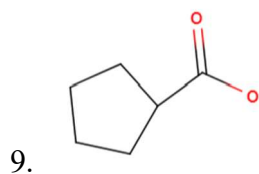
4. Draw a molecule with four carbons containing a carbonyl group. Circle the carbonyl group in your work.

5. Draw a molecule with four carbons containing a hydroxyl group. Circle the hydroxyl group in your work.

From the set of images, identify the

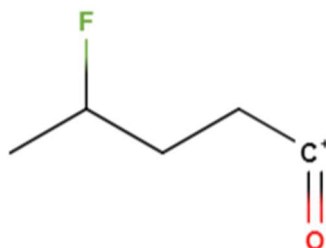
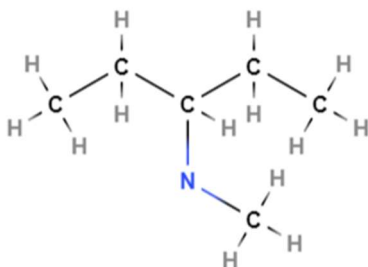
- a. Alcohol
- b. Carboxylic acid
- c. Ester
- d. Ketone
- e. I am not sure





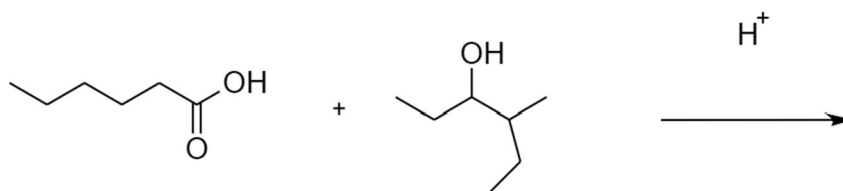
10. Calculate the formal charge on the carbon

11. Calculate the formal charge on the nitrogen. The nitrogen does have a full octet.

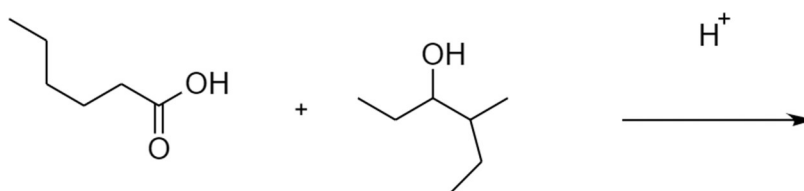


12. Circle areas with high electron density and place a square around areas with low electron density.

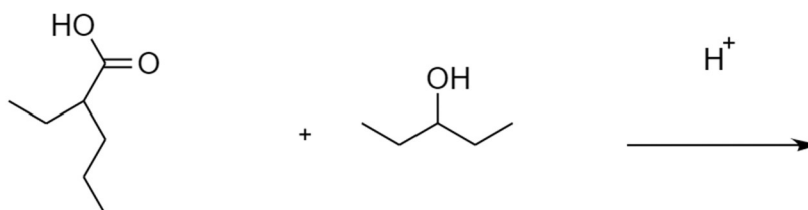
13. Draw the mechanism and product(s) of this reaction.



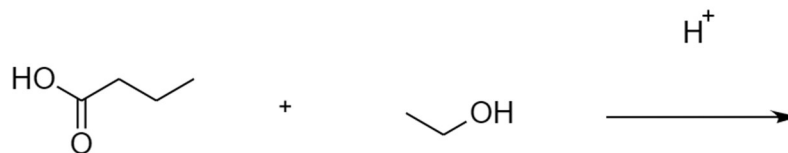
14. Draw the mechanism and product(s) of this reaction.



15. Draw the mechanism and product(s) of this reaction.



16. Draw the mechanism and product(s) of this reaction.



## APPENDIX B

### INTERVIEW QUESTIONS

Participants will be called one at a time in alphabetical order from the class roster. The participant and instructor will meet outside of the classroom in the hallway at a table. The instructor will ask the questions and record the responses to be transcribed later. Participants will be made aware of this.

“Good morning. How is your day going? I really appreciate your participation in this study so I want to thank you again. I am looking forward to sharing the results with you once it is completed. Ok, let’s get started if you are ready.

1. How did you feel about the entire unit, the content, MolView and your performance?
2. Did you find MolView to be difficult at any point? Why or why not?
3. Which type of model did you find more useful, 2D drawn models or 3D virtual models?
4. Are there challenges with either and if so, what are they? Explain.
5. Do you have a preference?
6. Was the 3D representation helpful in developing your understanding of formal charges and electronegativity? Did it make it more difficult to understand?
7. Do you think you understand why the reaction occurs at the sites it does?
8. How did you feel you performed on the written test compared to how you actually performed? Explain any discrepancies between the two if any.

9. Do you think the 3D representation hindered your performance?
10. If you performed as you expected, did the 3D representation activities help with your performance?
11. How did you feel you performed on the reaction mechanism questions compared to how you actually performed? Explain any discrepancies between the two if any.
12. Do you think the 3D representation hindered your performance?
13. If you performed as you expected, did the 3D representation activities help with your performance?
14. Could the 3D representation be useful to you in the future? (for other chemistry courses)
15. How did you approach this question?<sup>a</sup>
16. Can you tell me about the mechanistic arrows that you drew?<sup>a</sup>
17. Why are those the best electrons to push in this part of the reaction?
18. Does the formal charge of the atom change? How?
19. What does this mean?
20. What are the functional groups in the molecule?
21. Can you tell me more about your transition state structure?<sup>a</sup>
22. What do you think “transition state structure” means?<sup>a</sup>

## APPENDIX C

### SEGMENTS FROM THE ARTICULATION ASSESSMENT

Jon

Interviewer: Okay. Explain how you approach this problem to solve it through.

Jon: So, I see that there's an acid over here. This acid is willing to lose its hydrogen, and there's a high electron density area on the oxygen. It's double bonded to the carbon and the carboxylic acid. So, the electrons over there are going to be involved in trading for this hydrogen, but then this acid is now going to be more negative and willing to give up electrons because it is lost. So now, because we've bonded that hydrogen to the oxygen that already had two bonds, it has a positive formal charge. And because oxygen is really electronegative, it's not stable with a positive formal charge. So, it resonance moves that formal charge elsewhere in the atom, and then that double bond, the electrons that are involved in the double bond move to fill in the deficit that the oxygen is now under, and that leaves that deficit on the carbon. But now that there's a deficit on the carbon, that is an available bonding site for something else, which is where the alcohol comes in and the available electrons in the electron, that's region on the hydroxyl group of the alcohol that fills in that deficit

on the carbon. But in doing that, now you have a formal charge on the oxygen in the alcohol. And in order to solve that, because we have a whole bunch of alcohols, and we now have an alcohol that ends up with a carbon on either side of it, the hydrogen moves to a different alcohol in the molecule. And after that happens, you have, effectively, a positively charged oxygen in water on our molecule, which allows for it to really easily split from the group that forms our leaving group.

Charlie

Interviewer: "...can you tell me how did you approach this question in particular?

Charlie: So, I went back to what we learned. So, it started out with bringing in the acid, because that's the catalyst which makes the reaction possible and makes it easier, faster, and then you put that in... Okay, so for the first step with the acid, it is wanting to give up that hydrogen because it's an acid, and that's what the definition of an acid is. And then that oxygen with the pi bonds with the carbon is a really high electron dense region. So, it's a really good spot for that reaction to happen, to take up that proton from the acid. The second step with that oxygen, now there's a positive formal charge. Since it has that oxygen, that makes it outside of its normal bonding pattern, and there's resonance around that carbon. So, there's an electron deficient region. So, then the oxygen on the alcohol can come in and try and make it more stable.



Interviewer: Okay. All right. So, can you tell me about the mechanistic arrows that you drew and what they represent?

Charlie: So, the arrows, they represent electrons being transferred. The end that doesn't have an arrow on it, I think it's the tail end...Ok, the one that represents where the electrons are coming from. So, whether it's from, lone pairs on a molecule or from a pi, so those are where the electrons are coming from, and then the end of the arrow is where they're going to, forming a bond or creating a lone pair.

Gracie

Interviewer: All right, so what do you think happened at the reaction at this oxygen and at this carbon?

Gracie: So, the carbon has a positive formal charge. It doesn't have any lone pairs, and that's why it has a positive formal charge, because it's stable with four bonds and no lone pairs. However, it only has three bonds, and then the oxygen is stable because it has two bonds and two lone pairs. But the fact that there's another molecule within the reaction that has a negative formal charge, the acid catalyst that was used in the very beginning. It needs to come in somewhere. So, when it attacks the hydrogen, all the electrons were able to move over and make the carbon happy because it didn't have any, well, it had very little electron density to begin with, but then it slowly filled its shell and was able to become stable. And that's why at the product, there wasn't a formal charge on it on either molecule.

Interviewer: ...Are there any implications of it now having a zero-formal charge versus it having a positive formal charge?

Gracie: Having a positive formal charge would mean is much more likely for reaction to take place because it's electron deficient, so it would look for a source of electrons. But with a neutral formal charge, it would be much harder to have a reaction at that carbon.

Interviewer: Can you tell me more about your transition state structures walking us between steps two and step five?

Gracie: The carboxylic acid is essentially just the same as it was, but it has the oxygen in the carbonyl group, has a positive formal charge because it's bonded to hydrogen from the acid catalyst. And then the alcohol is oxygen from the alcohol that's still in the reaction is doing a nucleophilic attack on the carbon. And then once step two is done, it essentially becomes a huge molecule. Well, huge in the sense that we know it, that it combines together. There's two OH groups and the isopropyl group. And then the oxygen from one of the hydroxide groups attacks the hydrogen from the oxygen that has a formal charge and is able to leave with that. Because water makes a better leaving group than an alcohol would, then, well, water is formed and then the acid catalyst that was deprotonated from the first step is still hanging out in the solution. And then the big molecule, I guess, as we say, is pretty unstable as the carbon that's bonded to two oxygens has a positive formal charge. One of the oxygens has a hydrogen and it's able to go to the old acid catalyst, the base, the new conjugate base

is attacking the hydrogen that is bonded to one of the oxygens and so that it makes a double bond with the carbon and is able to make it a lot more stable than it was.”

Aston

Interviewer: Can you explain the mechanistic arrows that you drew?

Aston: Basically. It's just wherever the electrons need to move around the molecule. They will go to the spot that either has low electron density, where it would, such as carbocations, where the electrons were needed. From the alcohol, would go over to the carboxylic acid with the extra proton. But then, with the oxygens that were not overloaded but had a negative formal charge... they would move away from it. Such as whenever the water also leaves.