Using Effective Stereoscopic Molecular Model Visualizations in Undergraduate Classrooms

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Abstract

Chemistry students have difficulty understanding abstract scientific concepts of molecular structures. Physical molecular models have been used in class with some success, but this is not enough to support comprehension of key molecular concepts. Past research reports that scientific visualization using computer graphics has been useful for teaching and learning molecular properties. This paper describes a proposal for future research on the use of stereoscopic visualization of graphical molecular models to be applied in educational settings. Anaglyph projections (A type of stereoscopic display that is seen through low-cost glasses with red-cyan filters) were used in a pilot study to demonstrate the usefulness and efficacy (usability) of molecular anaglyphs in a computer lab. Further research will use anaglyphs of molecular models in a classroom. We will analyze whether anaglyphs are an effective tool to support molecular visualization for learning and teaching in combination with other teaching tools. System usability and student motivation will also be assessed.

1. Introduction

Undergraduate students generally have difficulty developing a conceptual understanding of chemical representations, including symbolic and molecular structures of Chemistry [1]. Empirical studies (e.g.[2]) have shown that many students do not easily understand the representations of molecules due to their scale (in the range of nm or pm), their abstract physico-chemical properties, and their intricate three-dimensional structure. Misconceptions often happen with the understanding of chemical bonding [3], a basic concept necessary to learn the nature of chemical reactions as well as properties of molecules, including boiling and melting points. Although students usually learn how to deal with molecular geometries using different formats (e.g., Fisher projections, Lewis structures, shorthand, etc.; Figure 1a), they still require to construct spatial reasoning and understand the three-dimensional arrangement of molecular structures [4, 5].

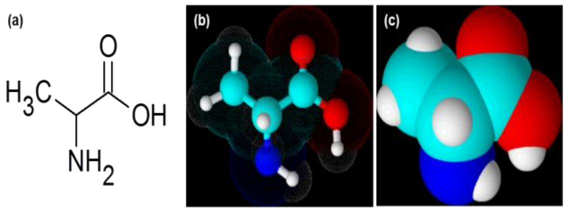

Figure 1. Molecular representations of glycine: a) bond-line; b) ball and stick; c) filled models (Created with ACD/ChemSketch version 12.0.)

Traditional teaching tools (e.g. the blackboard or plastic molecular models, such as the one showed in Figure 2) can be used to teach some general concepts about the structure of molecules, but they have certain limitations in terms of facilitating the understanding of very specific and precise properties related to the structure and dynamics of molecules. That is why students should rely on visual information, and such information should be displayed to the student in a practical and accessible way [6].

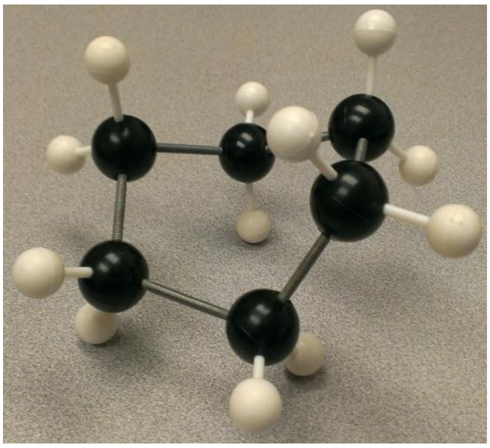

Figure 2. A Plastic (physical) molecular model representing hexane

The study and analysis of molecular structures and their properties have been conducted with fair success for some decades by visualizing graphical models of molecules in 3D (Figure 1). Most of these models have been shown in virtual environments (computer-generated three-dimensional spaces where a user can interact with the graphical representation) generally using desktop and laptop computers [7]. Molecular model visualization has also been carried out in a very limited way using mobile computing, such as the so-called smart phones. According to [8], molecular visualization on mobile devices may be useful to explore basic molecular structures of proteins, and this type of visualization can be used in academic conferences, informal meetings, brainstorming sessions and other meetings where there is no immediate access to a desktop computer.

2. Stereoscopy and Anaglyphs

Stereoscopy and can be very useful for supporting understanding of science concepts in education [9], particularly about molecular structure, since many molecular structure concepts rely on three-dimensional visual information, as demonstrated by [10]. Stereoscopy encompasses a number of visual techniques for creating or enhancing the illusion of depth in an image or computer graphics by means of stereopsis for binocular vision. Both of the 2D offset images used in stereoscopy are combined in the brain to give the perception of 3D depth. The human eyes of most adults are close to each other by approximately 5cm (2”). Every viewed object has a slightly different viewing angle in each eye. If two artificially-created images have the same angle difference (called deviation), and each eye sees the corresponding image, a visual spatial effect (3D illusion) is created [11].

The stereoscopy technique called anaglyph uses two color filters (generally red and cyan), one for each eye. The generated image for the left eye is generally red colored and the image for the right eye has a contrasting color such as blue, cyan or green [12]. The advantage of anaglyphs is that images or computer graphics used as anaglyphs are easy to create, use and distribute [16]. In addition, red-cyan glasses are cheaply available. Anaglyphs can also be projected onto a large screen using a conventional data projector [13]. Thus, low-budget schools can easily incorporate and use anaglyph technique in science classes. However, anaglyphs present some disadvantages. Some red/blue filters do not compensate the 250nm difference in the wave lengths of the red/blue colors. The red-cyan image can be blurry and ghosting can occur since the retinal focus differs from the one through the cyan filter. In addition, colored images can be difficult to display using the anaglyph technique. In consequence, visual fatigue may affect some users after a long period of anaglyph visualization.

The latter problems can be prevented and/or minimized by adequately creating the anaglyphs and testing them before they are regularly used in the classroom, and employing them for short periods of time, about 2-3 minutes. This can happen in-between the use of other types of educational materials or instructor explanations. Also, the successful creation and use of anaglyphs in the classroom should follow sound instructional design models such as the ADDIE model (see Figure 3), which is based on the Analyze, Design, Develop, Implement, and Evaluate phases [17]. Advantages of the ADDIE model include the development and improvement of prototypes of educational materials before their actual use in class, and a constant revision and testing of the materials during their design and development processes. During the Analysis phase, the instructor creates the lesson objectives on the educational anaglyphs, and identifies the learners' previous knowledge and skills regarding molecular structure. In the Design phase, the instructor (or the development team) plans and designs the user interfaces and prototypes, the lesson, and the instructional strategies. During the Development phase, the team develops the electronic materials, such as the computerized molecular models, the user interfaces (in case the team will not be using an already-developed molecular visualization program), and other supporting materials. In the Implementation phase the team develops a number of procedures for both the instructor and the learners, which include delivery of learning outcomes, method of delivery, and testing procedures. This phase includes training procedures on new software tools that describe how to use the molecular models and the molecular visualization software. The Evaluation phase includes formative (done during all phases) and summative (done at the end) evaluations and revisions on the design and the usability of the electronic materials, such as testing the molecular models and the molecular visualization software *in situ*, that is, in a computer classroom. Usability is a branch of computer science that measures how effective, efficient and pleasant to use a human-computer interface is. Past literature has shown that educational software designed with high usability generally improves learners' motivation and in turn facilitates learning [18].

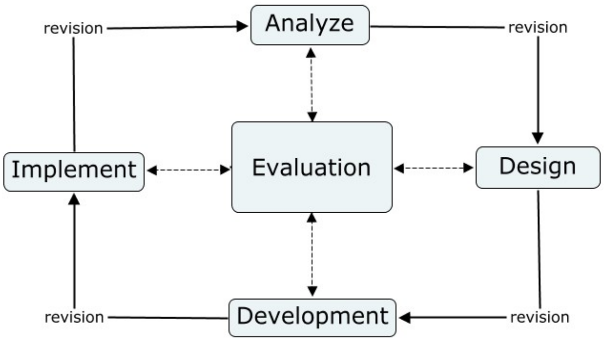

Figure 3. the ADDIE model (Source: Wikipedia).

In addition to instructional design, the development of educational anaglyphs should also follow strong learning theories, as explained in next section.

3. Learning Theories

John Sweller's Cognitive Load Theory [14] states that learning can be enhanced by improving presentation of information. The Cognitive Load Theory also indicates that our working memory is limited regarding the amount of information it can hold, thus we should provide students with didactic materials that facilitate and optimize their working memory processes. Learning requires working memory to be actively engaged in the processing and comprehension of instructional material to encode to-be-learned information into long term memory. In our case, we should adequately show molecular models to students with enhanced 3D depth trough anaglyphs and other spatial cues that may support working memory processes on the molecular structure and in turn facilitate learning. A related theory is the Cognitive Theory of Multimedia Learning [15], which also states that learning may be supported through the use of animations and other forms of electronic instructional materials. To put or our theory findings into practice, we devised a pilot usability test with anaglyphs and the molecular visualization software called PyMOL, described next.

4. Pilot Study

A pilot study was conducted with four computer science undergraduate students. They have had previous experience in watching anaglyph graphics, but they have not watched anaglyphs of molecular models before. The objectives of the pilot study was twofold:

- To test out and analyze the feasibility of anaglyphs of molecular models in an educational setting such as a computer lab or a classroom.
- To analyze students' first impressions on the use of anaglyph molecular models to be used in an educational setting.

4.1. Materials

Program PyMOL is an open source (free) molecular modeler that was used to display a molecule of Alanine (a common amino acid) to the participants. PyMOL allows the display of molecules as anaglyphs, enhancing their 3D structural perception. A screenshot of PyMOL is showed in Figure 4. The participants were wearing commercial carton glasses with red-cyan filters. The molecular model of Alanine was displayed on a 50" plasma TV (working as a computer monitor) using a laptop computer with Linux Ubuntu operating system and PyMOL installed on it. The pilot study was conducted in a computer lab especially dedicated for designing and developing video games used by computer science undergraduates.

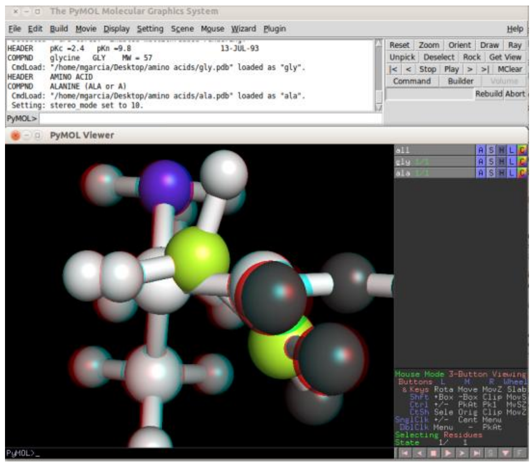

Figure 4. An anaglyph of molecule Alanine showed in PyMOL [19]

4.2. Procedure

The experimenter rotated and zoomed in and out the molecular model, explaining and showing the main structural features of the molecule while the participants watched the molecule using the anaglyph glasses. Figure 5 shows the complete set up and some of the participants watching the anaglyph.

Figure 5. A molecular model (anaglyph) displayed on a large computer monitor

4.3. Pilot Study Preliminary Results

Preliminary results showed positive feedback from the participants. Most of them thought the anaglyph can be really useful in a chemistry class. We found from the pilot study the following technical and logistic issues. We will need to address them when we run further studies with the molecular anaglyphs showed in a classroom:

- We need to rotate the molecular model slowly in order to avoid visualization dizziness and to keep the 3D depth effect.
- The molecular projection should be at least 2 meters apart from the first row of students in the classroom or lab.
- The lights of the computer lab or classroom where the anaglyphs are projected should be turned off in order to maximize the stereoscopic effect.
- The glasses with the red-cyan filters should be worn for small periods of time, for example between 1 and 3 minutes in between other activities that last longer, such as using a PowerPoint presentation. Using the glasses continuously for a long time may cause dizziness in some participants. Thus, the use of the anaglyph displays should be combined with other digital tools, such as a PowerPoint presentation or a video clip to avoid visual fatigue.
- A large computer monitor can be used for teaching molecular structure to a small number of students. We could see that even students seated at the extremes of the monitor could still easily perceive the stereoscopic effect of the anaglyph.
- The anaglyph technique is easy to set up. Also, it is a low-cost visualization technique (the carton glasses cost about one U.S. dollar each, and the molecular modeling program can be freely downloaded from the Internet). This can be really useful and convenient for schools with a limited budget.
- The anaglyph technique can efficiently support teaching of molecular models, provided that the anaglyphs are adequately used in combination with conventional teaching tools, such as physical models and/or PowerPoint presentations.

Our next step will be to test out the anaglyphs of the molecular model with organic chemistry and biochemistry students in a classroom, using a conventional data projector. We anticipate that this approach will help students understand the relationship between molecular structure and function not only for simple molecules such as amino acids (Figure 4), but also for complex proteins with quaternary structure, such as hemoglobin (Figure 6). We will use stereoscopic representations in combination with physical molecular models and PowerPoint presentations. We will measure aspects such as the system usability (system effectiveness, system efficacy and student satisfaction) and student motivation.

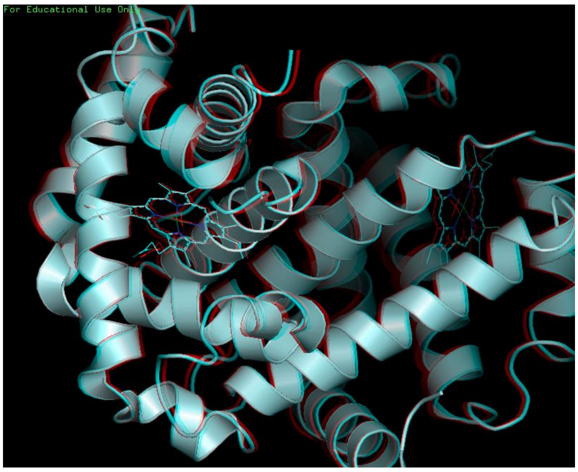

Figure 6. Anaglyph showing two β-subunits of oxygenated human hemoglobin, each tightly associated with a non-protein heme group (an Fe ion held in a porphyrin ring). The figure was generated with PyMOL [19]

5. Conclusions

Chemistry students have difficulty understanding abstract scientific concepts of structural properties of molecules. Physical molecular models have been used in class with some success, but it is not sufficient to support comprehension of key molecular concepts, such as bond length. Past research reports that computer-based scientific visualization has been useful for teaching and learning in chemistry, facilitating comprehension of abstract molecular properties, which are difficult to perceive through visualization of physical models alone. As [20] stated, a perceptual "trick" such as stereopsis is highly effective to support understanding of the three-dimensional properties of many molecular models, and electronic molecular models allow students to manipulate and visualize them easily, quickly and accurately.

In addition, to be effective, efficient and pleasant to use, computerized molecular visualizations should have high usability, and they should be designed and developed using a sound instructional design model such as the ADDIE (Analysis, Design, Development, Implementation and Evaluation) and follow strong educational theories.

This paper described a proposal for future research on the usability of stereoscopic visualization of graphical molecular models to be used in an educational setting, such as conventional classrooms. Anaglyph projections will be used to enhance the 3D perception of molecular models. The paper analyzed whether anaglyphs are an effective and usable tool to support learning and teaching of molecular visualization. An informal pilot study was conducted in a university computer lab to test out a simple molecular visualization as anaglyph. Results showed positive feedback from students who participated in the study. Also, the pilot study showed that anaglyph visualization presents some logistic and technical issues that need to be addressed prior and during the use of anaglyphs in a classroom. The anaglyph visualization technique is a very low-cost and useful tool for teaching and learning molecular structure that can be applied in a classroom or a computer lab with a minimum of computer settings and with an open source program such as PyMOL. Usability and learning issues will be addressed in future molecular visualization studies in a classroom with a data projector displaying molecular anaglyphs.

6. References

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