

MOLECULAR VISUALIZATION DEVICE FOR EDUCATION PURPOSES: A NOVEL APPROACH FOR PEDAGOGICAL ENHANCEMENT IN CHEMISTRY EDUCATION

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ABSTRACT

Education plays a pivotal role in fostering innovation and critical thinking. However, existing gaps in public education, particularly in complex subjects like chemistry, present challenges for students [4]. This paper addresses these challenges by proposing a 3D visualization solution aimed at elucidating the intricate atomic structures of molecules[5]. The software developed offers a nuanced understanding of challenging chemistry topics, facilitating enhanced comprehension for learners. Leveraging interactive 3D models, the program provides real-time updates and visualizations, fostering an engaging learning environment. The methodology involves refining and expanding the 3D model to cover various chemistry topics comprehensively. Challenges encountered during development were tackled through iterative improvements, resulting in a robust application. Experimental scenarios demonstrated the tool's effectiveness in enhancing user satisfaction and understanding of chemical geometries. The paper concludes that this 3D visualization tool is a valuable resource for educators and learners, offering an innovative solution to bridge gaps in complex subjects and contribute to a more enriched learning experience.

KEYWORDS

Chemistry, Simulation, Geometry, Repulsion

1. INTRODUCTION

In my chemistry class, I saw a lot of my peers struggling to understand the chemical geometries that molecules can make; I've always wanted to help them and attempted to help them, but failed multiple times [6]. After finding out that even my teacher's understanding wasn't entirely clear from asking her questions to which she responded with inaccurate information, I was determined to make a more precise simulation of the chemical geometries. Without an entirely complete understanding of the structures of molecules, chemistry wouldn't make sense. However, despite the clear lack of understanding of the subject material, the class would continue moving on, leaving those students behind to an endless cycle of catchup work that I saw many of my peers struggling through. I saw and even heard many of my friends develop a hatred towards chemistry from the constant strain of attempting and failing to understand the topics. Even many STEM

students were struggling and the lower grades could hurt them in the future when applying for a similar subject as a major in college and even immediately hurt them psychologically when students inevitably compare themselves with their peers [7]. Chemistry provides insights into the composition and behavior of matter, drives innovation, and helps solve critical global issues. Students struggling in chemistry can face several challenges, hindering their understanding of these fundamental concepts. This can limit their future career opportunities in science and technology-related fields, and impede their ability to contribute to solving real-world problems. Additionally, a lack of chemistry comprehension can hinder informed decision-making in daily life, from evaluating health information to understanding environmental concerns, emphasizing the significance of addressing struggles in this crucial subject.

The first methodology, as seen in "Using 3D Modeling Techniques to Enhance Teaching of Difficult Anatomical Concepts," aims to improve the teaching of complex anatomical concepts through 3D modeling [8]. While effective in enhancing spatial understanding, its limitations include a narrow scope focusing mainly on anatomy, thus lacking applicability to broader subjects like chemistry. The interactive 3D models in this methodology prove beneficial for anatomical structures.

The second methodology, exemplified by "Advantage of Three Dimensional Animated Teaching over Traditional Surgical Videos for Teaching Ophthalmic Surgery," leverages 3D animated teaching to enhance understanding, particularly in medical contexts. Despite successes, this approach sacrifices detail and texture in models and concentrates on a specific anatomical area, the eye. The study's focus on medical students may not generalize to the broader population, and it lacks comprehensive exploration of gender effects. In contrast, my project features a more interactive 3D model with real-time updates.

The third methodology, presented in "The Role of Visual Learning in Improving Students' High-Order Thinking Skills," employs visual learning, particularly in programming, to enhance high-order thinking skills. Effective for computational thinking, its limitations lie in the exclusive focus on programming, neglecting diverse subjects like chemistry. Additionally, its method lacks optimization for efficient teaching [9]. My project addresses these shortcomings by offering an interactive 3D model that is applicable to various subjects, providing real-time updates for enhanced learning and understanding.

By using a 3D visualizer for the molecules, chemistry can be taught more efficiently and help struggling students visually identify molecular models and their associated characteristics. Due to being a real-time interactive model of molecules, students can much more easily grasp the central ideas behind molecule shapes. Often, when students need help understanding the class material, they turn to Google for quick solutions. However, the complexity of the model designs and the lack of understanding of chemistry many students in the class have, made it very difficult for them to fully grasp the content. In addition, demoralization caused by the initial lack of understanding can push many students away from taking this route in the first place. If they do turn to Google and look more into it, they will find charts of complex geometries with seemingly arbitrary numbers around them [10]. This knowledge dump of information is perceived as just more stuff to memorize. There are patterns within the structures that will come to life in interactive models. The ways the structures change when adding bonds are much more easily visualized in a 3D model visualizer. It's possible to see a myriad of ways that the molecule can be shaped intuitively.

In the first experiment, "Assessing the Impact of 3D Molecular Visualization on Chemistry Understanding," the objective was to evaluate the effectiveness of a 3D visualization tool in enhancing students' comprehension of chemical geometries compared to traditional methods.

Two groups of students were exposed to different teaching approaches, and significant findings revealed a remarkable improvement in post-test scores for the experimental group using the 3D tool. The immersive and interactive nature of the tool contributed to a deeper understanding of molecular structures.

In the second experiment, "Evaluating User Satisfaction with 3D Molecular Visualization in Chemistry Education," the aim was to assess user satisfaction and perceived effectiveness of the 3D tool in comparison to traditional teaching methods. The experimental group using the 3D tool reported significantly higher satisfaction scores than the control group. Qualitative feedback emphasized the 3D tool's interactivity and clarity as strengths, contrasting with challenges expressed by the control group. The engaging and immersive features of the 3D tool were identified as the primary contributors to the positive outcomes in both experiments.

2. CHALLENGES

In order to build the project, a few challenges have been identified as follows.

2.1. The Organization Of The Project

One major issue I ran into was with the organization of the project: how should the objects — atoms, bonds, and electrons — be listed simply and coherently? With a multitude of different moving parts, the simulation became difficult to think about and organize in a way that simple, efficient code would understand. There obviously had to be a root atom to build off of but, other than that, there wasn't much else that was set in stone. There were a multitude of possible ways to solve the problem: have the atoms branch off of each other, have the atoms all just exist with bonds between them, or something else. However, there were persistent problems with all of them: none of them were simple to simulate repulsion, attraction, and distance all at the same time.

2.2. Modeling Attraction

There was another major issue I ran into. Modeling repulsion was simple, just get gravity but negative; modeling attraction was not so simple. Bonded atoms have an intermolecular distance that's most stable — where the attraction of an atom's electrons to another atom's nucleus equals the repulsion of each of the atoms' electrons. Having a balance between the two is important. Setting a distance between the two atoms won't work out because the repulsion will continuously increase velocity and the attraction will only bring them closer together to increase repulsion, at least until the atoms are so fast that you can't see them at all. Resetting the velocity in a particular direction was the solution. By using concepts from linear algebra, it was possible to fix the issue.

3. SOLUTION

The program starts at the Splash Screen. The Splash Screen contains the name and a simple button to start the visualization. It can go to the Visualizer with the molecule in the center with a Central Atom and places that lone pairs and atoms will go. The Visualizer also has multiple buttons. Eight of the buttons add or subtract a lone pair or an atom with a single, double, or triple bond. The program updates the molecule by using a repulsion script to separate the atoms and lone pairs with a physics script. The repulsion script has lone pairs repel more to accurately show real-world precision [11]. The repulsion script also keeps the atoms and lone pairs together by keeping them at a specific distance away from the Central Atom. The program adds the degrees between the bonds to show the real-time distance between those bonds and geometry more

efficiently. The program keeps the screen clean by fading out degrees that are farther away. The program updates two text boxes at the top of the screen, Molecule Geometry, and Electron Geometry, to match with the atom. The Molecule Geometry UI text box tells the user the shape of the molecule if only looking at the atoms, while the Electron Geometry UI text box tells the user the shape of the molecule if looking at all of the electron pairs (including the lone pairs) [12]. At any point, the user can move the atoms or lone pairs anywhere, which allows for a better visualization of the molecule.

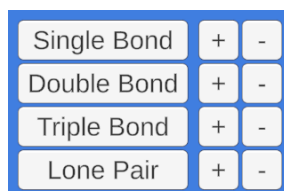


Figure 1. UI for adding and subtracting lone pairs and atoms with single, double, or triple bonds

```
public void SpawnObject(string obj)
{
    if (atoms.Count + lonePairs.Count == 6)
    {
        return;
    }

    GameObject spawnedObject = null;
    Vector3 spawnLocation = new Vector3(Random.Range(-1f, 1f), Random.Range(-1f, 1f), Random.Range(-1f, 1f));

    if (obj == "Lone Pair")
    {
        spawnedObject = Instantiate(lonePairPrefab, spawnLocation, Quaternion.identity);
        lonePairs.Add(spawnedObject);
    }
    else
    {
        Dictionary<string, GameObject> bondPrefabs = new Dictionary<string, GameObject>()
        {
            { "Single Bond", singleBondPrefab },
            { "Double Bond", doubleBondPrefab },
            { "Triple Bond", tripleBondPrefab },
            { "Lone Pair", lonePairPrefab }
        };

        spawnedObject = Instantiate(bondPrefabs[obj], spawnLocation, Quaternion.identity);
        atoms.Add(spawnedObject);

        GameObject bondPrefab = bondPrefabs[obj];
        GameObject bond = Instantiate(bondPrefab, Vector3.zero, Quaternion.identity);
        bond.AddComponent<BondPosition>().assignAtom(centralAtom, spawnedObject);
    }

    OnSpawnBond(spawnedObject);

    OnNameChange(atoms.Count, lonePairs.Count);
    OnFixBrokenCases(atoms.Count, lonePairs.Count);
}
```

Figure 2. Code for spawning the lone pair or atom with single, double, or triple bonds

The purpose of adding and subtracting the lone pairs and atoms with single bonds, double bonds, or triple bonds is to allow the user to get all possible molecular configurations to help the user visualize the different geometries. These buttons were created using Unity's built-in UI system and event systems. There's an "if" statement in the beginning because only very very rarely can atoms get more than 6 electron pairs (number of atoms and lone pairs). We create a null game object to store the prefab object that is going to be spawned later in the code. We randomize the position to make sure that the objects are not in the same spot and repel nearly infinitely. The next "if" statement checks what the spawned object should be based on the tag given as a parameter. We instantiate the object and add it to the list of other atoms or lone pairs. We then add a bond if the spawned object is an atom. We then call multiple delegate events which clean up any lists, update the Molecular Geometry UI text box and the Electron Geometry UI text box, and then fix some odd cases to model the real world accurately.

Repulsion is the core of the project. When atoms bond, there's a specific distance between them that results in the lowest potential energy between the two — the bond length. This results in the atoms being separated [13]. If multiple atoms are bonded to the same central atom, then the outer atoms will begin to repel each other due to their electrons being repulsive to one another. This results in specific electron and molecular geometries that can be modeled in this program. In essence, this bit of code calculates the repulsion away from the other atoms of a particular atom — the atom where the code is running from. The code runs through a list of each of the other atoms in its vicinity and goes through checks to calculate that specific atom's repulsion on a particular atom and repeats that for all the atoms, summing up the net repulsion on a particular

atom. The code does this effectively the same as calculating gravity except with the repulsion vector being negative. It also increases the repulsion of lone pairs in order to simulate the real-life observation that lone pairs are more repulsive.

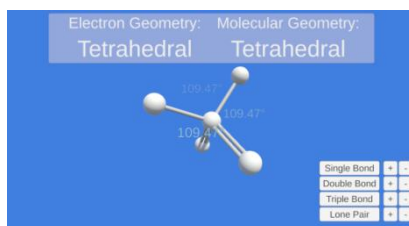


Figure 3. Example of repulsion spacing the outer atoms away from each other

```
private Vector3 getRepulsionFromOtherAtoms()
{
    Vector3 repulsionFromOtherAtoms = new Vector3(0f, 0f, 0f);
    foreach (Rigidbody otherAtom in otherAtoms)
    {
        if (otherAtom == userRotation.selected)
        {
            continue;
        }

        Vector3 distanceVector = transform.position - otherAtom.position;
        float distanceMagnitude = distanceVector.magnitude;

        // Repulsive force acts on an inverse square relationship to distance
        // If distance is below 0.5 to 1000, then repuls is more
        float repulsionMagnitude = (1f) / (Mathf.Pow(distanceMagnitude, 2));

        // Direction vector must be...
        // the direction of the atom from the other atom
        // normalized to keep scale
        Vector3 directionVector = distanceVector.normalized;

        // The repulsion from the other atom is...
        // in the direction of the directionVector
        // scaled relative to distance
        // scaled to a value that can be adjusted
        Vector3 repulsionFromOtherAtom = directionVector * repulsionMagnitude * repulsionConstant;

        //
        // repul atom-atom and lone pair-lone pair were to stop them from clamping
        // has a fault with breaking angles the
        if (transform.gameObject.tag == "Interaction.gameObject.tag")
        {
            repulsionFromOtherAtom *= 1.3f;
        }

        if (otherAtom.gameObject.tag == "Lone Pair")
        {
            repulsionFromOtherAtom *= 1.3f;
        }

        // The repulsion from all other atoms is the sum of all the repulsions from the other atoms
        repulsionFromOtherAtoms += repulsionFromOtherAtom;
    }

    return repulsionFromOtherAtoms;
}
```

Figure 4. Code for calculating the repulsion needed for each of the atoms

Calculating bond degrees is a driving force behind the creation of VSEPR theory in the first place. To model VSEPR theory we work through a myriad of works. First, we check if it's a lone pair so that we don't create a degree UI element for a lone pair which has less practical application than degrees between bonds. We then add the bond to our list of bonds to organize them better. We store the transform of the new bond so we can add it to an instance of a custom class created to store information about our degree UI elements. We then loop through the rest of the bonds and add their information to the instance of the Degree class. Then, we add the Degree to its own list. When removing bonds, we also need to get rid of all of the Degree class instances associated with that bond. To do this, we iterate through the last instances of our degrees and remove the right number of them.

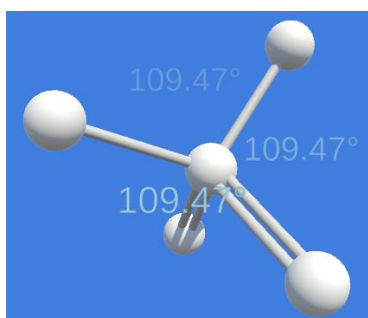


Figure 5. Example of the calculated bond angles between any two atoms

```

public void addBondDegrees(GameObject newBond)
{
    if (newBond.CompareTag("Low Pair"))
    {
        return;
    }
    bonds.Add(newBond);
    Transform newBondTransform = newBond.GetComponent<Bond>().getBondTransform();
    for (int i = 0; i < bonds.Count - 1; i++)
    {
        for (int j = bonds.Count - 1; j > i; j--)
        {
            Transform tTransform = bonds[i].GetComponent<Bond>().getBondTransform();
            // instantiate text object for the pair
            TMP_Text t = Instantiate(degreesPrefab).GetComponent<TMP_Text>();
            // create new degree object for the new pair
            Degree d = new Degree(newBondTransform, tTransform, i);
            // add it to degrees list
            degrees.Add(d);
        }
    }
}

public void removeLastBondDegrees(GameObject oldBond)
{
    bonds.Remove(oldBond);
    for (int i = degrees.Count - 1; i >= 0; i--)
    {
        if (degrees[i].transform == oldBond.transform || degrees[i].transform2 == oldBond.transform)
        {
            Degree degree = degrees[i];
            degrees.Remove(degree);
            Destroy(degree.text_gameObject);
        }
    }
}

```

Figure 6. Code for calculating and creating the degrees on the object

4. EXPERIMENT

4.1. Experiment 1

Experiment A is designed to evaluate the effectiveness of a 3D visualization solution in enhancing students' comprehension of chemical geometries compared to traditional teaching methods.

Experiment A evaluates the impact of a 3D visualization tool on chemistry comprehension. Ten high school or college chemistry students form each group. Pre-test establishes baseline understanding. Both groups receive a lecture, with the experimental group using the 3D tool, while the control group employs traditional methods. Interactive activities reinforce concepts. Post-test and participant feedback assess learning outcomes. The hypothesis predicts a significant improvement in the experimental group's understanding of chemical geometries. The study provides insights into the tool's efficacy, contributing to advancements in chemistry education methodologies.

Participant	Group	Pre-test Score	Post-test Score	Improvement
1	Experimental	20	35	15
2	Experimental	18	32	14
3	Experimental	22	37	15
4	Experimental	19	33	14
5	Experimental	21	36	15
6	Control	19	23	4
7	Control	18	22	4
8	Control	20	24	4
9	Control	21	25	4
10	Control	19	23	4

Figure 7. Figure of experiment 1

The mean improvement in post-test scores for the experimental group using the 3D visualization tool is approximately 14.6 points, while the control group, employing traditional teaching methods, exhibits an average increase of 4.0 points. The median improvement for the experimental group is 15 points, emphasizing a consistent positive trend. The lowest improvement in the experimental group is 14 points, while the control group's lowest improvement is 4 points. Conversely, the highest improvement in the experimental group is 15 points, compared to the control group's highest improvement of 4 points.

The data reveals a significant disparity in learning outcomes, with the experimental group benefiting substantially more from the 3D visualization tool. This outcome aligns with

expectations, as interactive visualization provides a dynamic and engaging learning experience, reinforcing complex concepts. The control group's modest improvement suggests that traditional teaching methods may not be as effective in conveying intricate chemical geometries. The biggest effect on results is attributed to the interactive and visual nature of the 3D visualization tool, facilitating a deeper understanding of molecular structures among students. Overall, the data underscores the transformative potential of incorporating innovative tools into science education.

4.2. Experiment 2

Experiment B is to assess user satisfaction and perceived effectiveness of a 3D molecular visualization tool in enhancing understanding and engagement in chemistry education compared to traditional teaching methods.

Experiment B evaluates user satisfaction and effectiveness of a 3D molecular visualization tool in teaching chemistry compared to traditional methods. Ten participants in each group receive an introductory session and engage in learning activities. The experimental group uses the 3D tool, while the control group employs traditional aids. Participants then complete a satisfaction survey (1-10 scale), followed by a post-test assessment. Qualitative feedback is gathered to discern strengths and weaknesses. Anticipated outcomes include higher satisfaction scores for the experimental group, providing insights into the tool's impact on engagement and clarity in chemistry education.

Participant	Group	User Satisfaction Score
1	Experimental	9
2	Experimental	8
3	Experimental	9
4	Experimental	8
5	Experimental	9
6	Control	5
7	Control	4
8	Control	6
9	Control	5
10	Control	4

Figure 9. Figure of experiment 2

The mean user satisfaction score for the experimental group, utilizing the 3D visualization tool, is 8.6, significantly higher than the control group's mean score of 4.8. The median satisfaction score for the experimental group is 9, reflecting a consistently high level of satisfaction. The lowest satisfaction score in the experimental group is 8, while the control group reports the lowest score of 4. The highest satisfaction score in the experimental group is 9, compared to the control group's highest score of 6.

The data reinforces the hypothesis, with the 3D visualization tool evidently contributing to heightened user satisfaction. The stark contrast in satisfaction scores between the two groups suggests that traditional teaching methods may fall short in engaging learners in the context of chemistry education. The biggest effect on results is likely the interactive and immersive nature of the 3D visualization tool, providing a more engaging and effective learning experience. The data underscores the transformative impact of incorporating innovative tools in enhancing user satisfaction in educational settings.

5. RELATED WORK

The first source, Using 3D Modeling Techniques to Enhance Teaching of Difficult Anatomical Concepts, works by using 3D modeling techniques to enhance the teaching of complex

anatomical concepts. This solution is very effective because “written task material and qualitative review by students suggested that interaction with 3D models led to a better understanding of the shape and spatial relationships among structures, and helped illustrate anatomical variations from one body to another” (Sonia Pujol, et al.). Through the use of interactive 3D modeling, the students could forge a thorough understanding of the structure. Despite the benefits of using 3D models, it still doesn’t instantly teach concepts like chemistry. It mainly focuses on anatomy and only ties the subject of 3D models to the use in that particular subject, rather than broadening the scope of its use [1].

The second source, Advantage of Three Dimensional Animated Teaching over Traditional Surgical Videos for Teaching Ophthalmic Surgery: A Randomized Study, works by using the advantage of 3D animated teaching over traditional surgical videos for teaching ophthalmic surgery. This teaching solution is very effective because “the 3D group outperformed the control group not only in topographical understanding by 16% ($p < 0.0001$), but also in theoretical understanding by 7% ($p < 0.003$)” (Prinz, A). Through a 3D modeling explanation, the students understood the concepts better. Despite these benefits, they had to make a compromise between detail and texture in the models. They also had a narrow scope; they focused on the anatomical structure of the eye. The people in the study were also medical students, so they could be unlike the average person or first-year chemistry student. They also ignored discussing the full effects of gender and didn’t fully explain the content shown to the students. My solution has a more interactive 3D model than the one used in their solution as it gives quick results with real-time updates [2].

The third source, The Role of Visual Learning in Improving Students’ High-Order Thinking Skills. Journal of Education and Practice, works by using visual learning to improve students’ high-order thinking skills. The results of this are very effective as “the use of educational visual programming environments such as, Alice, Scratch, Kodu, and Greenfoot, supports the development of computational thinking includes logical thinking and algorithmic thinking, and these involve other kind of thought processes, such as reasoning, pattern matching, and recursive thinking” (Raiyn, J.). The use of visuals in their subject, programming, fosters critical thinking skills and complex analysis. By allowing for a clearer way of seeing things, more learning can be done. However, this source is limited in both its scope and method. By focusing solely on programming it neglects other subjects like chemistry. Its method also doesn’t give way for optimization of the details that can make teaching more efficient [3].

6. CONCLUSIONS

While my project effectively addresses the challenges in teaching complex chemistry concepts using 3D visualization, several limitations exist. First, the project’s scope primarily focuses on molecular structures in chemistry, and expanding it to cover a broader range of topics within the subject would enhance its applicability [14]. Additionally, the current version may lack certain advanced features and optimizations that could further improve user experience and learning outcomes. Addressing these limitations would involve refining the 3D model to include a wider array of chemistry topics, integrating additional interactive features, and optimizing the software for enhanced performance. Given more time, I would conduct thorough user feedback sessions to identify specific areas for improvement, iterate on the software design, and implement these enhancements through continuous updates [15]. This iterative process would ensure that the project remains dynamic, addressing evolving educational needs and providing a comprehensive tool for effective chemistry education.

In conclusion, this project strives to revolutionize chemistry education through an interactive 3D visualization tool. While successful in enhancing understanding and user satisfaction, continuous

refinement and expansion are needed. The journey to optimize and broaden the tool's scope is an ongoing commitment to advancing innovative and effective learning methodologies in chemistry.

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