Creative Molecular Model Design for Chemistry Edutainment

Wanwan Li
wanwan@usf.edu
University of South Florida
Tampa, Florida, USA

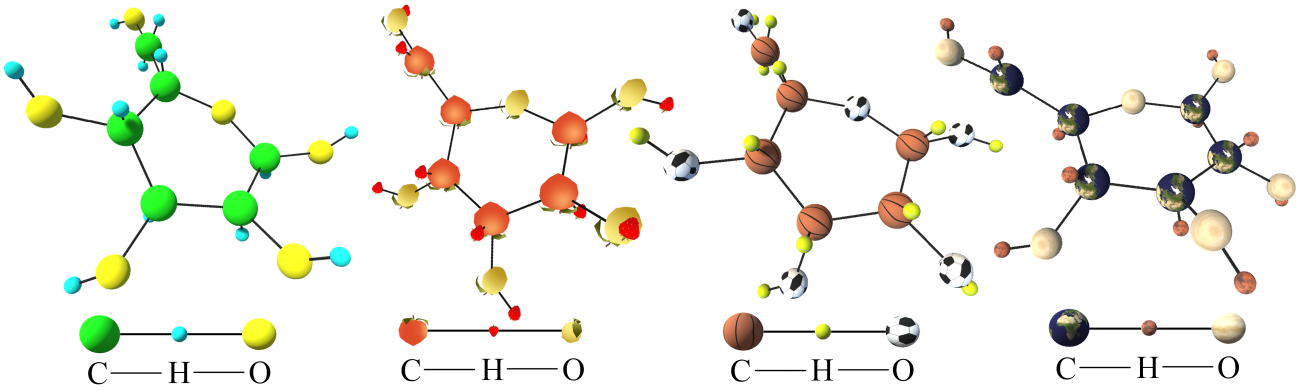

Figure 1: This figure shows an example that how a creative molecular model design is applied to chemistry edutainment using our proposed interactive user interface. In this example, we simulate and visualize the molecular chemical structure of Beta-D-Glucose ($C_6H_{12}O_6$) using an electric field energy optimization approach with different creative design styles including ball-stick style, fruit style, sport style, and planet style. This result shows the scalability of our proposed approach in designing creative molecules with arbitrary types of structures and various kinds of styles.

ABSTRACT

Since 3D molecular structure visualization is important for chemistry education, lots of successful works have been focused on molecular visualization. However, most of the existing research works consider the pre-defined types of chemical bonds and reassembling various kinds of bounds together to construct a 3D molecular structure using the standard ball-and-stick model. Although, this approach is good enough to visualize realistic molecular structures, it losses the generality to reveal the mechanism that how atoms are formed into a molecule from electrical explanations during the molecule design process. At the same time, no existing research works have explored how to generalize this visualization technique by introducing the entertainment elements in children's chemistry education. Therefore, in this paper, we propose a novel approach to visualize molecular structure in 3D space by minimizing the electric field energy where the optimization steps yield a realistic explanation that how a molecular structure is formed in nature, helping the students understand more about the dynamic properties of molecules. In the meantime, we apply our technique to creative molecular model design for chemistry edutainment.

CCS CONCEPTS

• **Computing methodologies** → **Scientific Applications**; **Multimedia Interaction**.

KEYWORDS

molecular formula, molecular structure, electric field energy, chemistry, edutainment.

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1 INTRODUCTION

As one of the most popular branches of computational chemistry [7, 14, 16, 26], molecule structure visualizations [2, 6, 19, 21, 22] have been widely studied by researchers nowadays. Understanding the molecule structures is the key issue for researchers and students to get a deeper insight into chemical reactions and molecular dynamics [1]. Since the early days, open source tool for the visualization and analysis of molecular structures such as Visual Molecular Dynamics (VMD) [13], gOpenMol [15], qMol [4], web application [8], and UCSF Chimera [23], etc. have been attracting most of the computational researchers and result in lost of successful visualizations and applications in chemistry education [3, 10, 18]. Later on, more advanced technologies in molecule structure visualizations were proposed. Sekercioglu et al. [24] proposed a mass-spring system [5, 12, 17] for molecular modeling yielding satisfactory results. Razer Hydra controllers-based interactive Molecular Modeling tool has been developed by [25] for scientific researchers. Hoksza et al. [11] developed a molecular structure visualization tool called MolArt that provides an interactive environment to present protein

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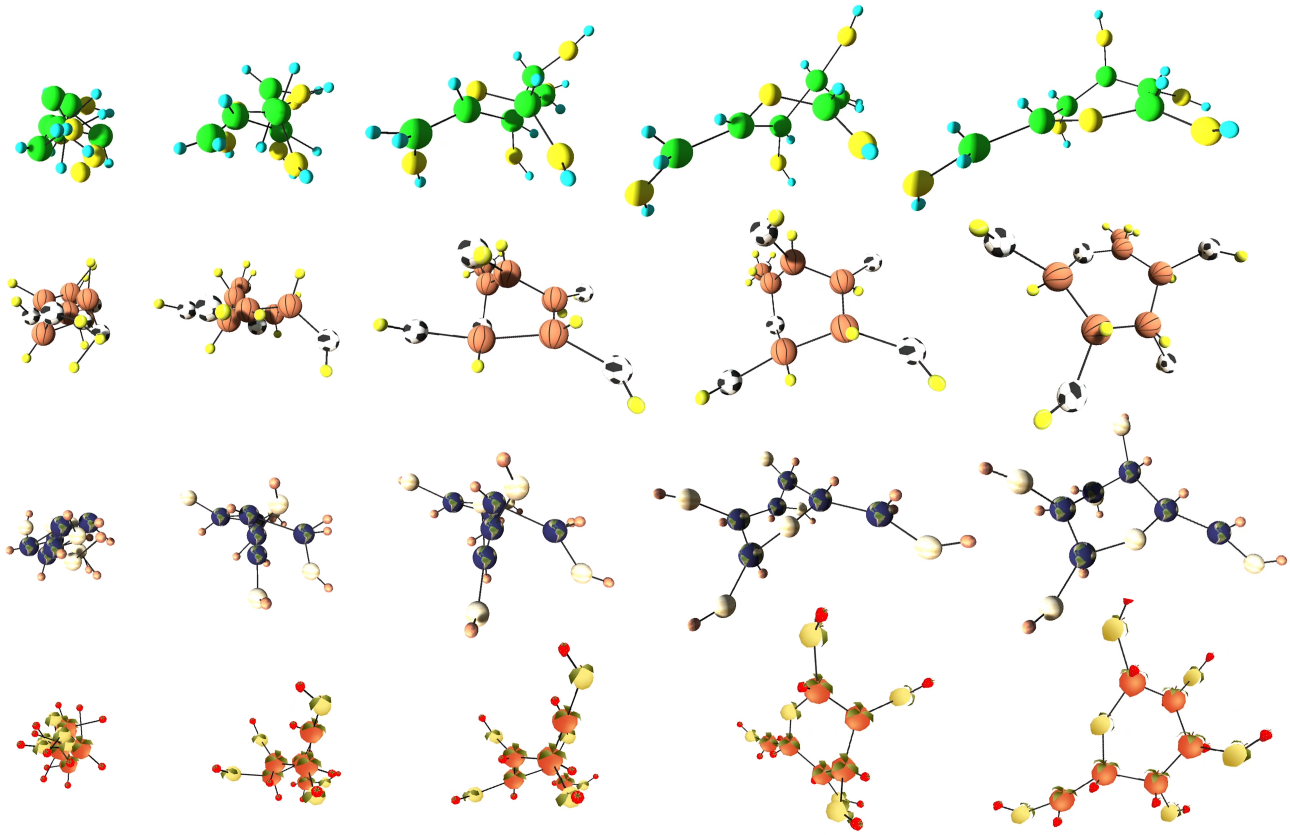

Figure 2: Optimization process.

structures. Recently, as new technologies in advanced immersive hardware display devices become mature and democratic, virtual reality(VR) and augmented reality(AR) platforms have been explored for immersive interactive environments for molecular modeling and visualization. For example, Goddard et al. [6] proposed a VR system for molecular visualization which contains three VR applications including ChimeraX, AltPDB, and Molecular Zoo for analyzing molecular structures and teaching young students characteristics of biomolecules. Muller et al. [20] presented an interactive molecular visualization platform for augmented reality using HoloLens. All these successful works address that molecular visualization plays an important role in computational chemistry and proved that recent new technologies in display hardware have been changing the way that how molecular visualizations take place.

However, most of the existing research works have been focused on pre-defined types of common chemical bonds and reassembling various kinds of bounds together to construct a 3D molecular structure. For example, Chem3D[28] [27] allows the users to set up the bonds type, bonds angles, and bond length so that the atoms can be assembled together instantly after a mouse click. Even Chem3D, like most other common molecule visualization tools, molecular dynamics (MD) [9] is implemented to simulate the oscillations of constructed molecules. Although, existing software is good enough to visualize realistic molecular structures and mimic the molecular dynamics caused by the electric forces, it losses the generality to reveal the mechanism that how atoms are formed into a molecule from electrical explanations. At the same time, no existing research works have explored how to generalize this visualization technique by introducing the entertainment elements in children's chemistry education. Therefore, in this paper, we propose a novel approach to visualize molecular structure in 3D space by minimizing the electric field energy, which is the source of the molecular forces within the molecule on the atoms' level. Therefore, the simulation process is the optimization process proposed by our approach, presenting a realistic explanation that how a molecular structure is formed in nature. Such a process can help the students understand more about the dynamic properties of molecules that inspire them with the ideas of more generally defined "molecules" that may or may not exists in the real world. In the meantime, we apply our technique to creative molecular model design for chemistry edutainment such as using different 3D models to render the molecules including ball-stick style, fruit style, sport style, and planet style, etc. Major contributions of our presented work include:

- We propose a novel research topic about devising an interactive user interface for supporting creative molecular model design for chemistry edutainment.

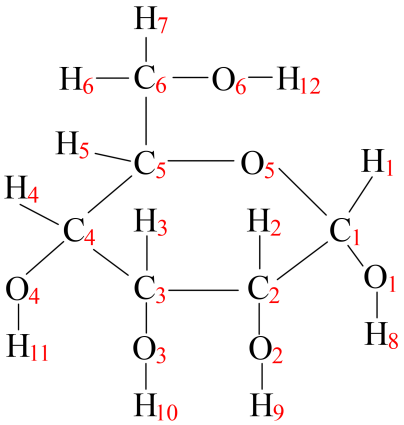

Figure 3: Structural formula of $C_6H_{12}O_6$.

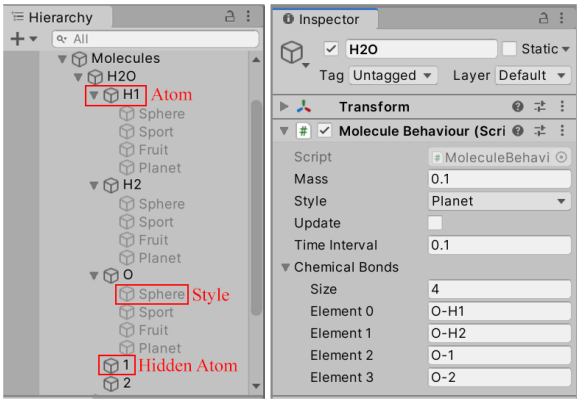

Figure 4: Unity3D editor user interface.

- We propose and implement an electric field energy optimization-based approach to simulate arbitrary molecular chemical structures defined by the user.
- We demonstrate and validate the results of our approach through numerical results on different types of creative molecular model designs. Please refer to the supplementary video https://youtu.be/jrD7QbN4AmA for more details.

2 TECHNICAL APPROACH

Figure 2 shows the optimization process of our technical approach for simulating the molecular structure in 3D space by minimizing the electric field energy. In this example, we use the molecular structure of Beta-D-Glucose ($C_6H_{12}O_6$) as shown in Figure 3 using an electric field energy optimization approach. Different columns in Figure 2 are corresponding to different iterations during the optimization and different rows are presenting the results with different creative design styles including ball-stick style, fruit style, sport style, and planet style. From the leftmost column to the rightmost column, as the iteration increases, the 3D molecule structures are expanded from a cluster of randomly generated atoms into a stable molecular structure in the end which is the same chemical structure specified in the molecular formula as shown in Figure 1. Let electric field energy defined as $E(Q, B)$, where $Q = \{q_1, q_2, ..., q_N\}$ are the electric charge of N atoms in the molecule and $B = \{(i, j)|1 \le i \le N, 1 \le j \le N, i \ne j\}$ are the chemical bonds in the molecule, our approach is implemented by solving this molecular electric field energy minimization problem:

$$E(Q, B) = k_1 \sum_{i=1}^{N} \sum_{j=1}^{N} \frac{q_i q_j}{r_{ij}^2} - k_2 \sum_{(i,j)\in B} r_{ij}, \tag{1}$$

where we empirically set $k_1 = 0.2$, $k_2 = 1.0$, $q_i = q_j = 0.2$, and $r_{i,j}$ denotes the distance between atom i and atom j. After solving Equation 1 by introducing the position vectors of the atoms as $\{\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_N\}$ and masses of atoms as $\{m_1, m_2, ..., m_N\}$, given an arbitrary random position in the 3D space for each molecule at t_0 which is denoted as $\mathbf{x}_i(t_0)$, then we have the position of arbitrary atom i at time t which is $\mathbf{x}_i(t)$ by dissecting the position updates into three parts, mathematically, $\mathbf{x}_i(t) = \mathbf{x}_i(t_0) + \Delta\mathbf{x}_i(t)' + \Delta\mathbf{x}_i(t)''$. Figure 5 illustrate the dissection of the position updates. where, $\Delta\mathbf{x}_i(t)'$ calculates the composite pushing force between atoms that is caused by electronic force and $\Delta\mathbf{x}_i(t)''$ calculates the pulling force between atoms caused by the chemical bounds between atoms that results in the . In this case of H_2O, there are two hidden atoms of H in the molecule design to represent the equivalent electron cloud, where $\Delta\mathbf{x}_i(t)'$ is:

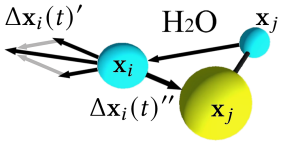

Figure 5: Position update.

$$\Delta\mathbf{x}_i(t)' = \frac{k_1 q_i}{m_i} \sum_{j=1}^{N} \int_0^t \left(\frac{\mathbf{x}_i - \mathbf{x}_j}{|\mathbf{x}_i - \mathbf{x}_j|^3} \right) q_j \mathrm{d}t, \tag{2}$$

and $\Delta\mathbf{x}_i(t)''$ is calculated as:

$$\Delta\mathbf{x}_i(t)'' = -\frac{k_2}{m_i} \sum_{(i,j)\in B} \int_0^t (\mathbf{x}_i - \mathbf{x}_j)\, \mathrm{d}t, \tag{3}$$

where we empirically set mass $m_i = m_j = 0.1$.

3 USER INTERFACE

We design a series of numerical experiments to validate our proposed approach using Unity 3D Game Engine. Figure 4 shows our proposed creative molecule design interface on Unity Editor. The "Hierarchy" window (left) shows the game objects of 3D molecules. In this example, the designed molecule is H_2O. Under the molecule, there are five atoms game object in the children game objects of H_2O molecule, they are H_1, H_2, O, 1, and 2 respectively. At here, atom 1 and atom 2 are two hidden atoms to approximate the virtual electron clouds. Therefore, there are no children game objects under the hidden atoms. Using our proposed optimization approach, interactions between visible and hidden atoms help the optimizer to generate a H_2O molecule with the chemical bonds at a 104.5° angle rather than 180.0° (Note that 180.0° is the case for missing hidden atoms where two H atoms directly push each other on a straight line without other force interactions). But for atoms H_1, H_2, and O, four each atom, they have four different children game objects representing different different types of creative molecule designs,

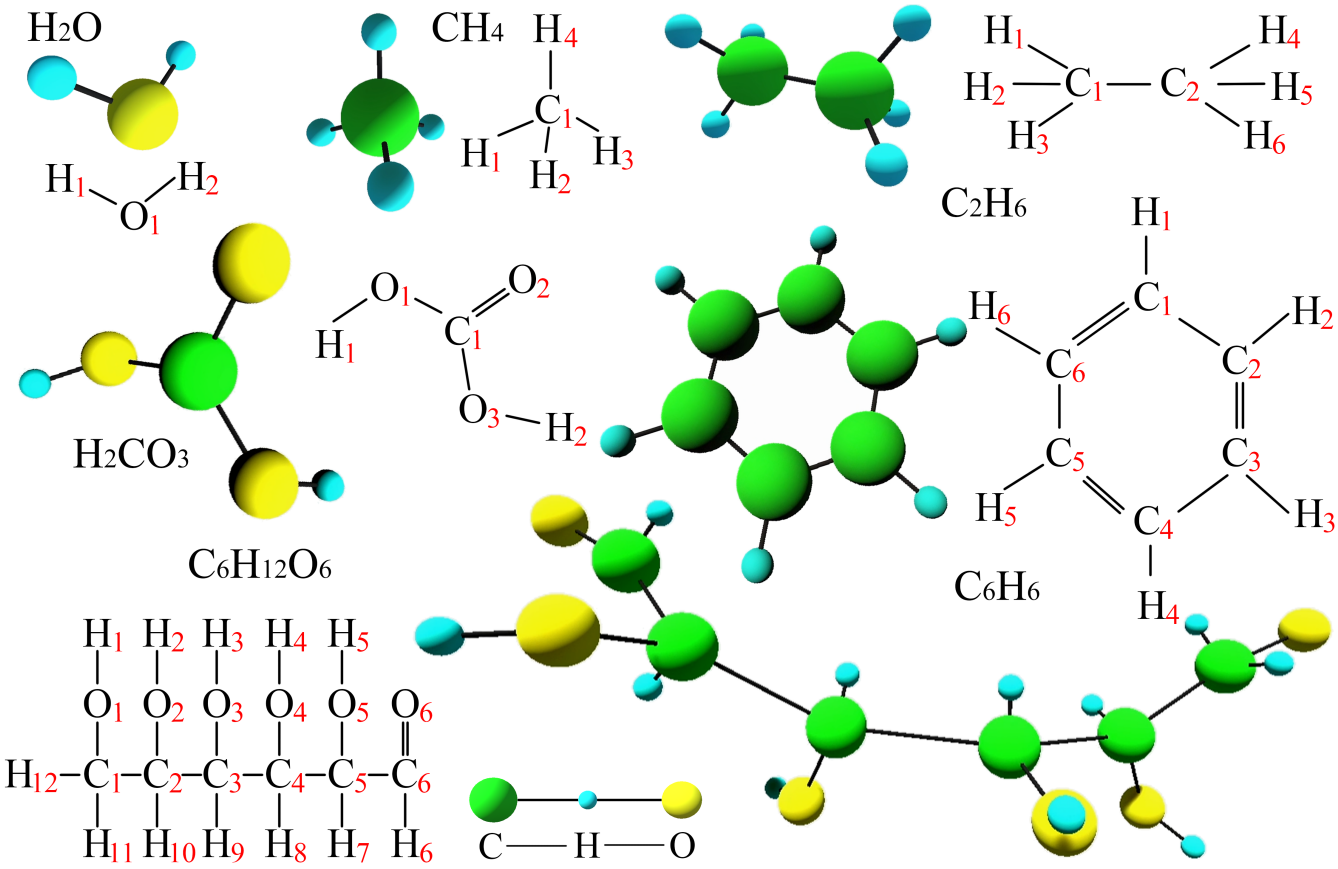

Figure 6: Experiment result: sphere style. This figure shows the molecule design using sphere style where atom Carbon *C*s' color is green, atom Hydrogen *H*s s' color is cyan, and atom Oxygen *O*s' color is yellow.

they are: sphere, sport, fruit, and planet respectively. We are showing that more general types or styles can be designed here, more details please refer to the supplementary video. The "Inspector" window (right) shows the Molecule Behaviour drag-drop interface. After the user specifies the chemical bonds in H_2O (they are $O-H_1$, $O-H_2$, $O-1$, and $O-2$ respectively), our Molecule Behaviour C# script automatically generate the H_2O molecule using our proposed optimization approach whose process is shown in Figure 2.

4 EXPERIMENT RESULTS

We design different molecules in different styles using the interface proposed in previous section. In this experiment, we explore our creative molecule design interface by designing six different kinds of molecules, they are the molecule of Water H_2O, Methane CH_4, Ethane C_2H_6, Carbonic acid H_2CO_3, Benzene C_6H_6, and D-(+)-Glucose $C_6H_{12}O_6$, respectively. Figure 6-9 shows the detailed experimental results of the creative molecule design using different styles. Figure 6 shows the molecule design using sphere style where atom Carbon *C*s' color is green, atom Hydrogen *H*s s' color is cyan, and atom Oxygen *O*s' color is yellow. Figure 7 shows the creative molecule design using sports style where atom Carbon *C*s are represented by basketballs, atom Hydrogen *H*s are represented by tennis, and atom Oxygen *O*s are represented by soccer. Figure 8 shows the creative molecule design using planet style where atom Carbon *C*s are represented by Earth, atom Hydrogen *H*s are represented by Mars, and atom Oxygen *O*s are represented by Venus. Figure 9 shows the creative molecule design using fruit style where atom Carbon *C*s are represented by oranges, atom Hydrogen *H*s are represented by strawberries, and atom Oxygen *O*s are represented by lemons. For each result, the corresponding chemical structural formulas are presented near its corresponding molecules. As we can tell from this experimental results, after the designer specifies the 3D models for each atom using different styles and specify the chemical bonds of the of each molecule, the final 3D modelcle model are generated automatically by solving our proposed optimization equations in previous sections. For example, the generated Methane CH_4 molecule is automatically generated as a 3D pyramid where each angle between two adjacent chemical bonds is 109.5° which is close to the 104.5° of the water molecule H_2O. We also generated the Ethane C_2H_6 molecule with the same chemical bonds angle of 109.5°. Different from Methane and Ethane, we generated

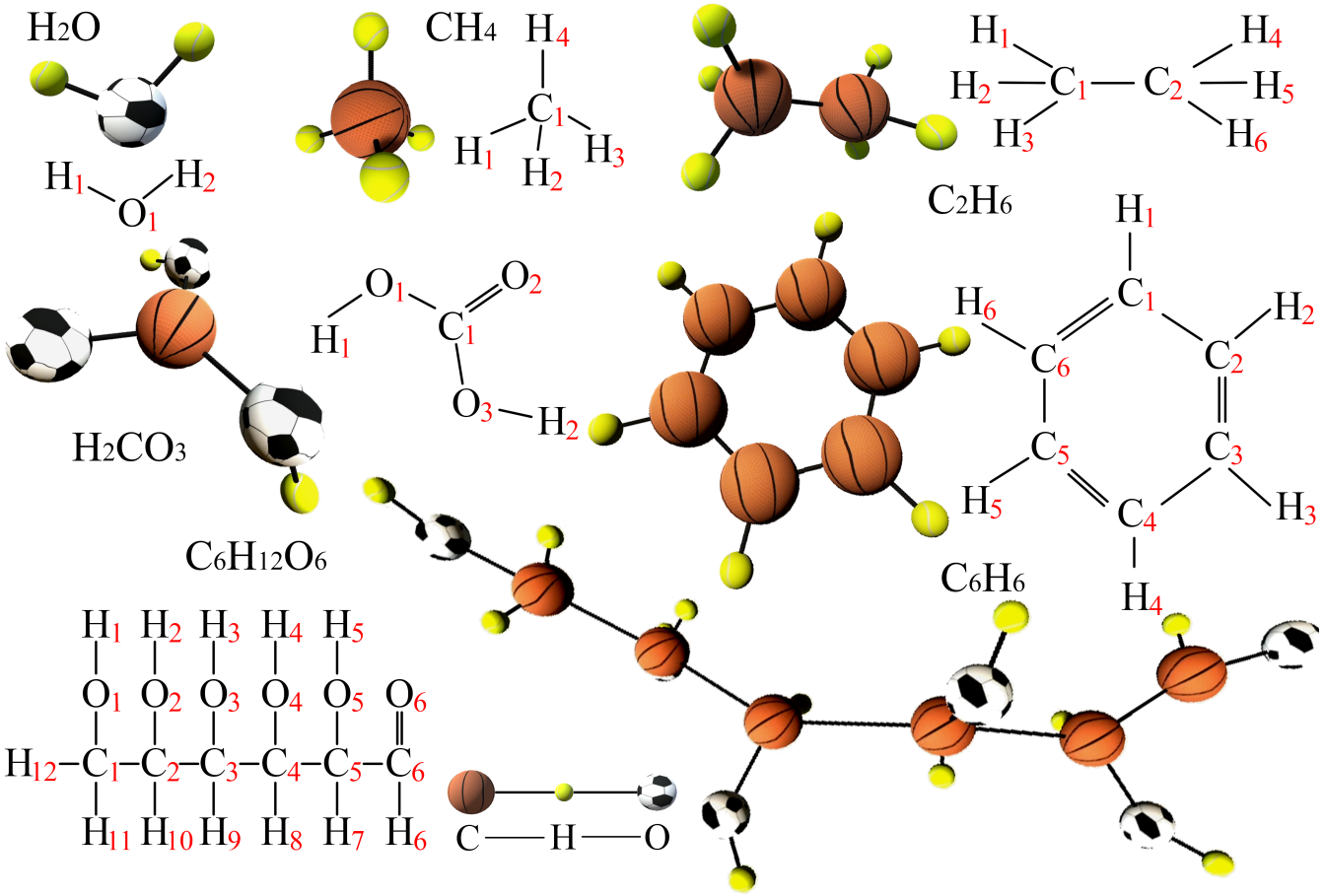

Figure 7: Experiment result: sports style. This figure shows the creative molecule design using sports style where atom Carbon *C*s are represented by basketballs, atom Hydrogen *H*s are represented by tennis, and atom Oxygen *O*s are represented by soccer.

the Benzene C_6H_6 molecule automatically with the 120° degrees around each carbon-Hydrogen bond and carbon-carbon bond and forms a hexagon circle. Similarly, we generate the Monosaccharide D-(+)-Glucose $C_6H_{12}O_6$ molecule structure approximate to the real structure which likes like a linear structure (indeed, more looks like a centipede). However, this structure is way different from the molecular structure of Beta-D-Glucose ($C_6H_{12}O_6$) where there is a hexagon circle inside itself more like the Benzene C_6H_6 molecule. In conclusion, all the above results validate the effectiveness of our approach to generate realistic molecule structures in real-time and can be generalized into different styles of atoms.

5 CONCLUSION

In this paper, we propose a novel approach to visualize molecular structure in 3D space by minimizing the electric field energy where the optimization steps yield a realistic explanation that how a molecular structure is formed in nature, helping the students understand more about the dynamic properties of molecules. In the meantime, we apply our technique to creative molecular model design for chemistry edutainment. Through a series of numerical experiments, we show how a creative molecular model design is applied to chemistry edutainment using our proposed interactive user interface. For example, we simulate and visualize the molecular chemical structure of Beta-D-Glucose ($C_6H_{12}O_6$) (in Figure 1) using an electric field energy optimization approach with different creative design styles including ball-stick style, fruit style, sport style, and planet style. All numerical results show the scalability of our proposed approach in generating arbitrary molecule structures and custom styles creatively. This provides the potential to apply our approach in chemistry edutainment which is a hot research topic for computer scientists to explore with.

Future Work. However, during the experimental process, we realize there are still some limitations within our proposed approach. For example, even though our approach can automatically synthesize realistic and creative molecule structures in real-time, however, there is still a missing statistical study to show how significantly our approach can speed up the creative molecule design process. Therefore, it is necessary to invite a group of users to design a 3D model of molecules using our proposed approach or design similar tasks in their preferred interactive interface or 3D design platforms.

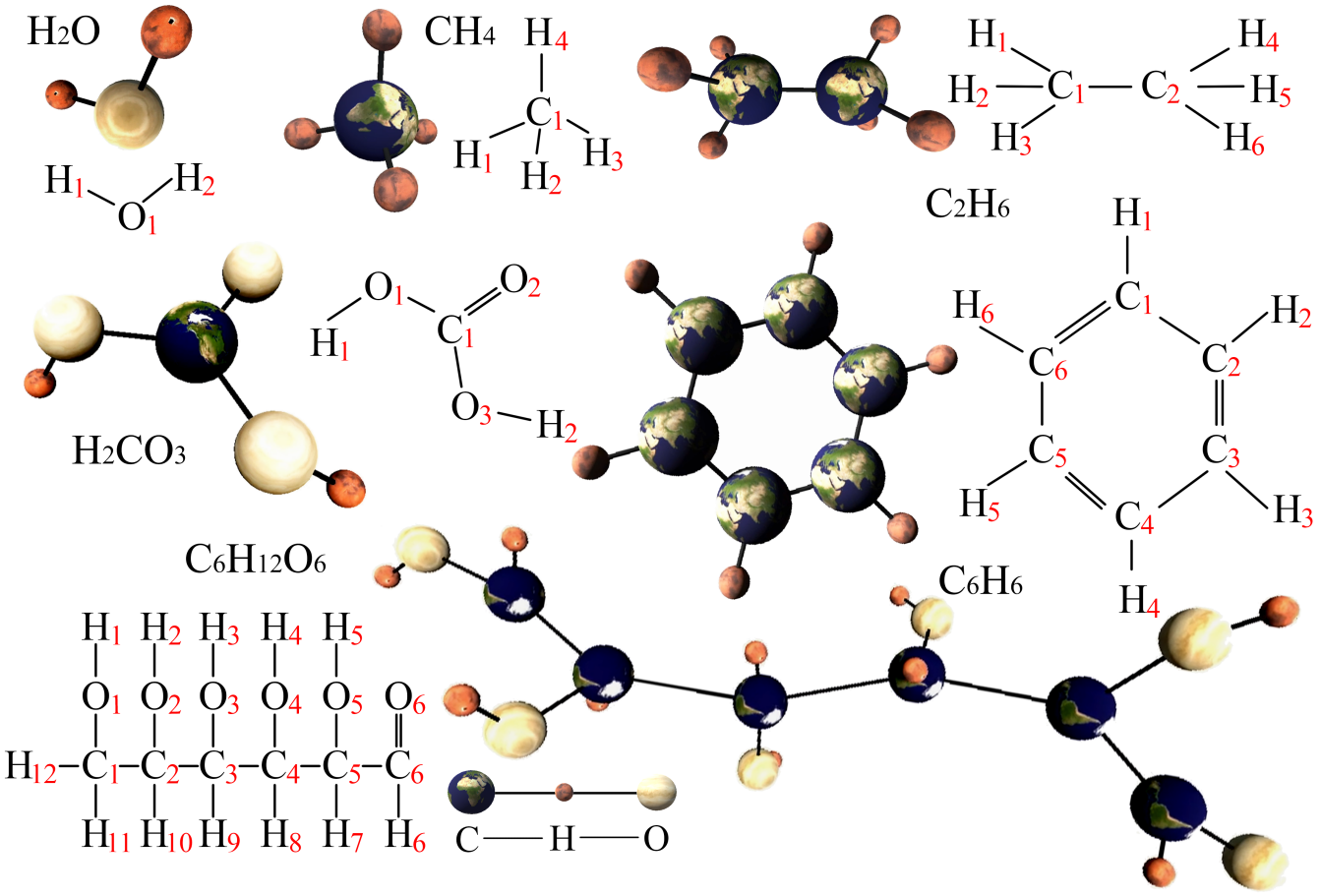

Figure 8: Experiment result: planet style. This figure shows the creative molecule design using planet style where atom Carbon *C*s are represented by Earth, atom Hydrogen *H*s are represented by Mars, and atom Oxygen *O*s are represented by Venus.

And take that group as a control group, to be compared with the group which is using our proposed interface according to the time and efforts spent by each group respectively.

On the other hand, more complex molecule structures need to be tested on our interface, although we show the effectiveness of generating a couple of different types of molecule structures which include complex structures such as Beta-D-Glucose ($C_6H_{12}O_6$) and D-(+)-Glucose $C_6H_{12}O_6$ which are already very complicated, however, more complicated ones such as DNA structures are still not tested. Therefore, our proposed approach can be only a promising prototype of design creative molecule structures, more studies are welcome in this reach direction.

A more important one, the reason we are choosing Unity3D editor as the 3D game engine for proposing our interface is because of the feature of Unity3D as it is easy to be transformed into eXtended Reality (XR) platforms such as Virtual Reality (VR), Augmented Reality (AR), and Mixed Reality (MR) which provide an immersive interactive experience for the users and players. However, we have not tested these interfaces for augmenting our approach to immersive environments, this provides another opening opportunity for researchers to explore further upon our proposed approach. This validates the value that is potentially delivered by our work.

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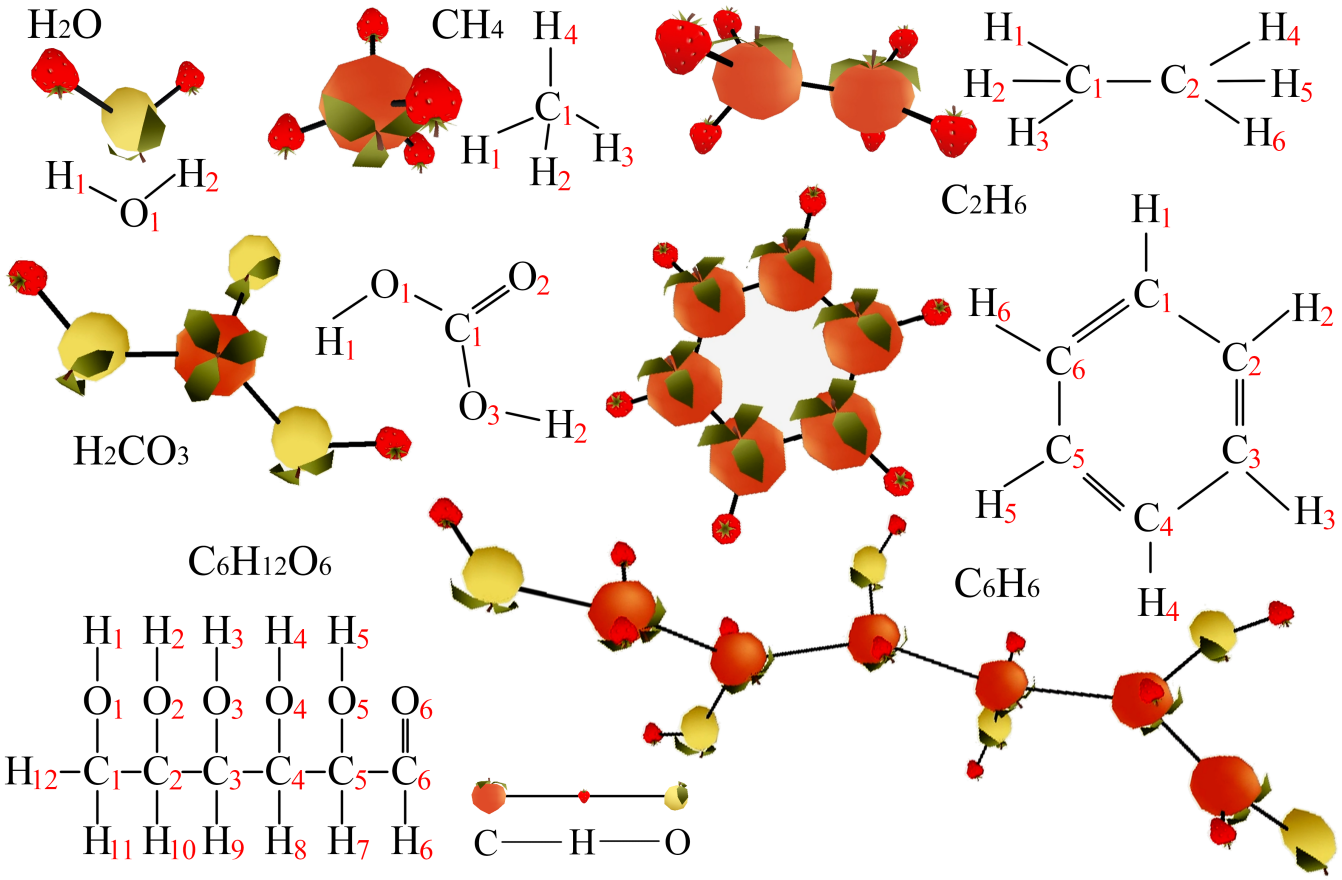

Figure 9: Experiment result: fruit style. This figure shows the creative molecule design using fruit style where atom Carbon *C*s are represented by oranges, atom Hydrogen *H*s are represented by strawberries, atom Oxygen *O*s are represented by lemons.

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