

## **Augmented Reality for teaching spatial relations**

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**Patrick Maier**, Technische Universität München, Germany

**Gudrun Klinker**, Technische Universität München, Germany

**Marcus Tönnis**, Technische Universität München, Germany

**Abstract:** This paper describes an approach for increasing the understanding and ease the learning of chemistry for students by visualizing and controlling virtual models of molecules in a intuitive way. With the Help of Augmented Reality, we developed a tool with the name Augmented Chemical Reactions. This program visualizes models of molecules rendered to a camera picture at the position of special markers hold in the hands of the users. The intuitive controlling of the position and orientation of the molecules is done by moving and rotating the markers in front of a camera, so the virtual objects behave as they would have been manipulated themselves. For a better understanding of the subject of chemistry, Augmented Chemical Reactions also shows the dynamic deformation of molecules when they come close to each other. Here the users can have a better view on certain behaviours between molecules. This program has the potential to increase the understanding and ease learning chemistry because of its intuitive controlling of the 3D structure of molecules. In the same way that Augmented Chemical Reactions can help students, it also has the potential to speed up the process of designing new molecules. Scientists can inspect the created molecules and see, if they meet the spatial requirements for specific reactions. This approach prevents time consuming reactions in the laboratory to create those molecules and test them for their desired attributes.

## **1 Introduction**

Many students have problems learning and understanding chemistry. This can be, because they can not imagine the spatial structure of the molecules which they are taught. The problem is, that teachers only have a two dimensional representation of the chemical molecules on the blackboard or on their slides. Understanding chemistry depends on understanding the spatial structure of the chemical parts. If the 3D understanding of the chemical structures is not given, the students have difficulties understanding certain behaviors of molecules. To understand why a specific chemical reaction behaves in a special manner and not in another way, there is the need to know the spatial arrangement of the atoms in a molecule. Some atoms could lie in the middle of a molecule and therefore can not be bound to an atom of another molecule from the outside because

of the repulsive forces from the surrounding atoms. If the spatial structure and dynamic behaviour of chemical molecules is conveyed to the students, chemical processes and chemistry per se could be better understood. Although there are many existing programs to visualize the molecules in 3D on a two dimensional screen, interactive schemes for rotating or moving the 3D objects are not intuitive. With the help of Augmented Reality, users can manipulate the virtual 3D objects in the computer in an simple and more intuitive way. As a result, Augmented Reality has the potential to improve the understanding of the spatial structure of a molecule. To achieve this, we have built a visualization tool to present and control molecules created with other. The new idea of this program is to show the dynamic behaviour in the interaction between molecules. Students can see the molecules deform when they approach each other.

## 2 Augmented Reality

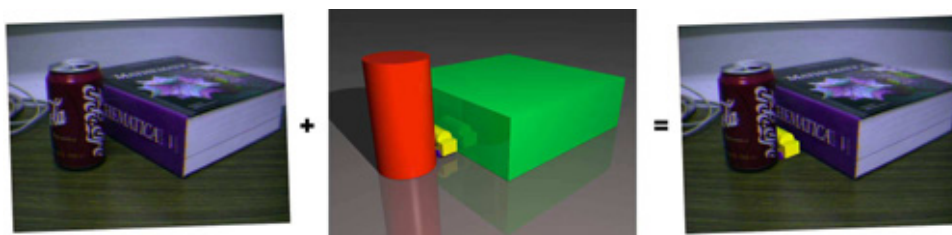


Figure 1: Basics of Augmented Reality

Augmented Reality (AR) is a newly emerging technology by which a user's view of the real world is augmented with additional information from a computer model. With mobile, wearable computers, users can access information without having to leave their work place. They can overlay the information three-dimensionally on the real world, manipulate and examine real objects and simultaneously receive additional information about them or the task at hand. Exploiting people's visual and spatial skills to navigate in a three-dimensional world, Augmented Reality thus constitutes a particularly promising new user interface paradigm. Figure 1 shows the basic concept of Augmented Reality. Additionally to the real world with its objects (here: a book, a can and a table), virtual objects such as the small yellow object in the second image can be rendered, such that they fit exactly to the real world image. When combining these images, the yellow object is integrated in the picture of the real world at its desired position. This generates the impression that the yellow object is an object of the real world. For Augmented Reality, this procedure has to be performed in real-time, such that a user can interact

with the real objects and the camera without losing the 3D connection to the virtual object.



Figure 2: Example of a marker

This technique requires tracking of the camera and the real objects, in order for the computer to know the positions of the real objects. With this information the virtual objects can be rendered exactly at the desired position in the picture of the camera. Tracking can be done with several systems. A common way of getting the data is using a marker tracker system, which takes a picture from a webcam, tries to find special patterns which represent markers (Figure 2). The position and rotation of the marker relative to the webcam is calculated with computer vision algorithms. Two main systems are AR-ToolKit (Kato & Billinghurst, 1999) and UbiTrack (Huber, Pustka, Keitler, Florian, & Klinker, 2007). This data is then passed to the Augmented Chemical Reactions application that uses this to calculate and control the molecules.

### **3 Related Work**

There are few supporting tools in education that use Augmented Reality. In mechanics education, Hannes Kaufmann et al. presented an augmented reality application named PhysicsPlayground (Kaufmann & Meyer, 2008). It uses a recent physics engine developed for the PC gaming market to simulate physical experiments in the domain of mechanics in real time. Students are enabled to actively build own experiments and study them in a three-dimensional virtual world. A variety of tools are provided to analyze forces, mass, paths and other properties of objects before, during and after experiments. Innovative teaching content is presented that exploits the

strengths of our immersive virtual environment. PhysicsPlayground serves as an example of how current technologies can be combined to deliver a new quality in physics education. To increase the learning effectiveness in chemistry education, Morten Fjeld et al. built Augmented Chemistry (Fjeld et al., 2007), an application that uses a tangible user interface for organic chemistry education. They compared learning effectiveness and user acceptance of Augmented Chemistry (AC) versus the more traditional ball-and-stick model. Learning effectiveness results were almost the same for both learning environments. User preference and rankings, using NASATLX and SUMI, showed stronger differences and they decided to focus mainly on improving these aspects in a re-design of the AC system. For enhanced interaction, keyboard-free system configuration, and internal/external database access, a graphical user interface has been incorporated into the tangible user interface. Three-dimensional rendering has also been improved using shadows and related effects, thereby enhancing depth perception. The re-designed Augmented Chemistry system was then compared to the old system by a small qualitative user study. This user study showed an improvement in subjective opinions on the system's ease of use and ease of learning.

Further related work was done by (Fjeld, Juchli, & Voegtli, 2003), (Fjeld & Voegtli, 2002), (Chen, 2006), (Kaufmann & Dünser, 2007).

Suzanne Weghorst et al. worked on a system to directly create physical 3D models of molecules, which are overlaid with additional information such as electrostatic fields (Weghorst, 2003). Recent studies are made by Eliana Medina et al. with static molecules to help students learn biochemistry (Medina, Chen, & Weghorst, 2007).

## **4 Augmented Chemical Reactions**

We have designed and implemented Augmented Chemical Reactions, a visualization program for chemical molecules. With this tool, it is possible to inspect molecules in an intuitive way. Chemists only have to create models of the desired molecules in their preferred application and load them into the Augmented Chemical Reactions program a cheap webcam and markers (Figure 2) are required, which are easily self made by printing a special pattern on a piece of paper. The program has two configuration modes. The first mode is for users who do not want to configure the system but simply start using it with predefined settings. This is, for example, for a group of students, who are given a special task to do. There is a second, expert mode, in which users can configure the whole system as seen in figure 3. In this mode users can chose a file, defining the structure of a molecule and assign it to a marker (Figure 2).

When holding this marker in the field of view of the webcam, the molecule model, created by the chemist and loaded into the program, is rendered on

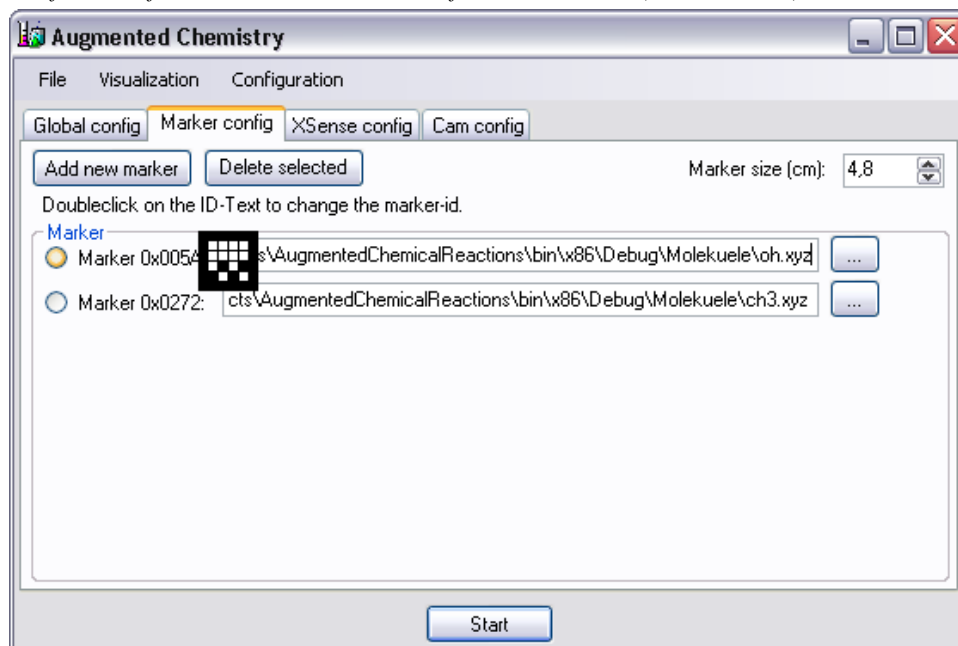


Figure 3: Assign markers with files that describe molecules

top of the marker in the webcam picture on the screen (Figure 4(a)). Because the system calculates the position and orientation of the marker from the webcam picture using computer vision algorithms, the molecule is drawn in the picture as if it were there in real life. With this technique it is possible to inspect the molecule from all sides as long as the marker is seen by the webcam. Defining more markers and assigning them with additional molecules (Figure 4(b)), allows visualizing and interacting with more molecules at the same time. With multiple markers, each controlling one molecule and the simulation turned on, the reaction of those molecules with each other is visualized. When the distance from an atom in one molecule to an atom in another molecule is small enough and the atoms have the ability to bind, a possible bond (represented by a transparent cylinder connecting those two atoms) is drawn and the molecules are starting to deform due to the forces between the molecules (Figure 5(a)). Figure 5(b) shows additional transparent cylinders drawn between the molecules, when there are more potential bonds. Here the students can see why chemical reactions happen in a certain way, according to the spatial structure of the molecules.

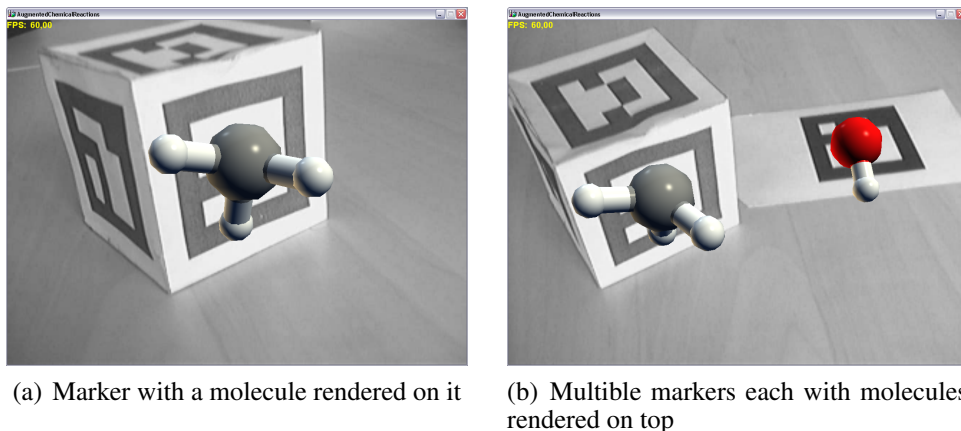


Figure 4: Augmented markers

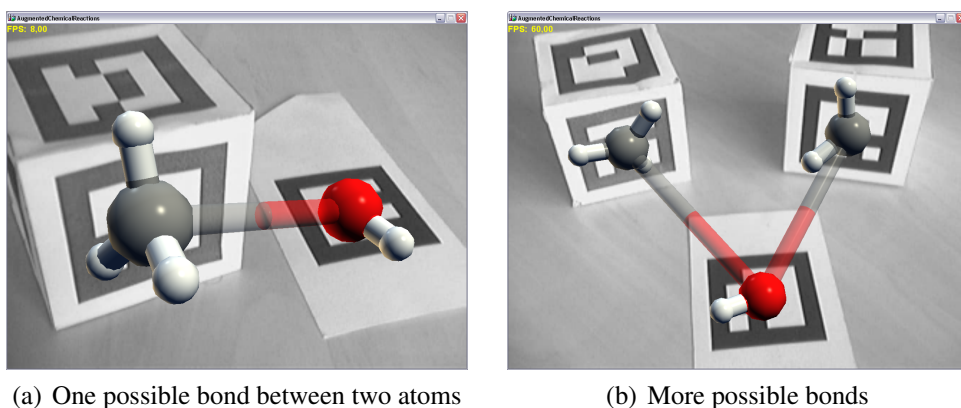


Figure 5: Molecules reacting with each other

#### 4.1 *New opportunities for teaching*

This application offers new opportunities for teaching and education. Students are no longer confronted only with the 2D representations of the chemical structures. They additionally have the option to inspect the molecules from every point of view. This intuitive controlling of the molecules is achieved by rotating and moving real objects (markers) rather than with keyboard and mouse. Especially for users who are not so familiar with rotating 3D objects, controlling by keyboard and mouse is difficult. In addition to inspecting the molecules, students can also control the interaction of two or more molecules with each other. When molecules come close to each other and finally react, the users can see the deformation of the molecules.

## **4.2 New opportunities for science**

For scientists the design of new molecules, such as new catalysts, is currently a time consuming task. When they design a new catalyst for a special reaction, they develop this possible molecule, and create it in the laboratory. It will take some days to generate the desired molecule. After that, the newly created catalyst is tested to see whether it has the requested attributes. Potentially, the chemists have to redo the whole process if they determine that the built catalyst does not have these attributes.

With Augmented Chemical Reactions, the scientists can easily see if the designed catalyst has the desired spatial structure to react with another molecule. If the designed catalyst does not fulfill the criteria, the molecule can be modified without the loss of time due to creating it in the laboratory.

## **5 Future Work**

Future work now has to determine, which gestures and user input methods to interact with the molecules are easy and intuitive to use. If for example it is necessary to use more than two molecules at the same time with more than two markers, it will be difficult to control it with the two hands of one person. There may be a need of other gestures to control more than two molecules. Further more, interactive facilities are needed that help building molecules from fragments and single atoms. Along with this comes the need to select a particular possible bond when more than one possible bonds are displayed to the user.

## **6 Conclusion**

Augmented Chemical Reactions could increase the understanding of chemistry as well as decrease the fear and reserved attitude in respect of the subject of chemistry, because it shows the spatial relations between molecules and their resulting reaction. It could be accepted by the students because of the new way of controlling and interacting with models of molecules in a playful way. It has the potential to speed up the process of developing and designing new molecules for scientists, when time consuming work in the laboratory is replaced by validating the designed molecules in a early stage.

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