

Augmented Chemical Reactions: An Augmented Reality Tool to support Chemistry Teaching

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Abstract—This demonstration shows an Augmented Reality tool to support teaching chemistry. The understanding of spacial relations in and between molecules is an essential part that has to be understood by students to learn chemistry. As nowadays the techniques to show and simulate molecular behaviors get faster and better, 3D applications to show the molecules become more and more popular also in schools. Augmented Chemical Reactions is an application that shows the 3D spatial structure of molecules as well as the dynamics of the atoms in and between molecules. This application does not use the commonly used 3D user interface of mice and keyboards to move and rotate the virtual objects but it makes use of an intuitive 3D user interface. This 3D User interface is an direct manipulation user interface using the augmented reality technique. With this user interface it enables the users to better understand the spacial structure of the shown geometries.

I. 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 normally have a two dimensional representation of the chemical molecules on the blackboard or on their slides. Understanding chemistry also 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 behavior 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 a simple and more intuitive way. We have shown [1] that the direct manipulation of an virtual object by using Augmented Reality improve the understanding of the spatial structure of a molecule more than using a 3D user interface with mouse and keyboard. To achieve this, we have built a visualization tool to

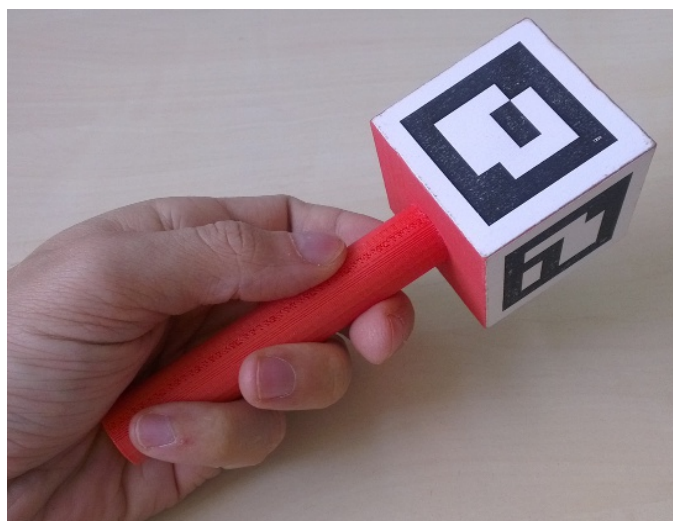


Fig. 1. This device is tracked by a computer with a webcam. It is used as a 3D input device for direct manipulation.

present and control molecules as well as show the dynamics in and between molecules. Students can inspect molecules as well as see the molecules deform when they approach each other.

II. AUGMENTED CHEMICAL REACTIONS

To combine the visualization of complex structures and the advantages of direct manipulating physical objects, *Augmented Chemistry* [2] and *Augmented Chemical Reactions* [3], [4] have been introduced. Both systems use Augmented Reality to deliver a direct manipulation 3D user interface to control the position and orientation of the virtual objects.

Generally speaking, Augmented Reality adds virtual information or objects interactively and in realtime to the real world, generating the impression that the added information is part of the physical world. To this end, the application *Augmented Chemical Reactions* employs a physical cube with a handle that is textured on all sides with black and white patterns (Figure 1). In a typical setup, a student holds the cube by the handle and manipulates it while sitting at a desk in front of a monitor (Figure 3). A webcam records the scene with the cube, and *Augmented Chemical Reactions* uses a marker

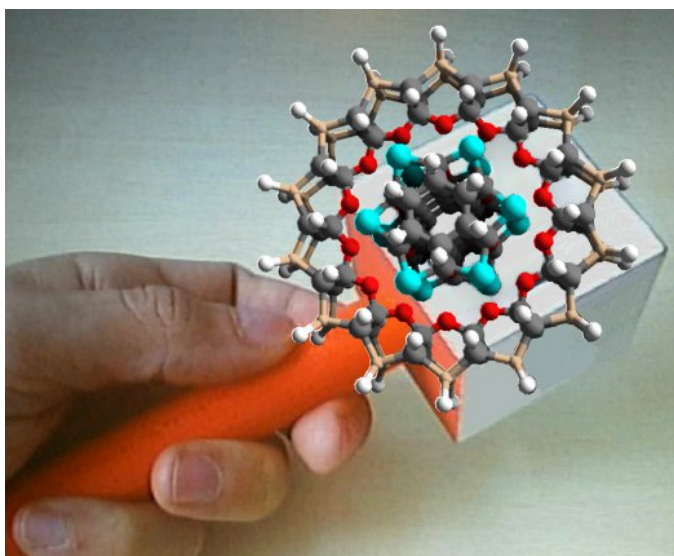


Fig. 2. Augmentation of a molecule on top of the marker cube.



Fig. 3. Computer setup for the *Augmented Chemical Reactions* application, using a webcam a physical cube on a handle and a monitor. The keyboard that is required to cycle through a set of molecules is not shown.

tracking algorithm similar to the AR-toolkit [5], [6] to detect and recognize the currently visible patterns on the cube.

According to the size and deformation of the patterns, the algorithm calculates their position and orientation relative to the webcam – and thus the pose of the cube and handle. With this information, the virtual molecule can be drawn on top of the webcam image, leading to the illusion, that the molecule is attached to the cube (Figure 2). The virtual molecule moves in unison with the physical cube. This is a three-dimensional direct manipulation user interface.

To be as flexible as possible, the application can associate any molecule that is stored in a Protein Database file (*.pdb) with the physical markers (Figure 4). Even more, the application supports various displaying methods as stereo on two screens, stereo head-mounted displays and ambient occlusion. It also can be used as a front-end to a molecular dynamics simulation to show the dynamics in and between the molecules and simultaneously interact with the molecules.

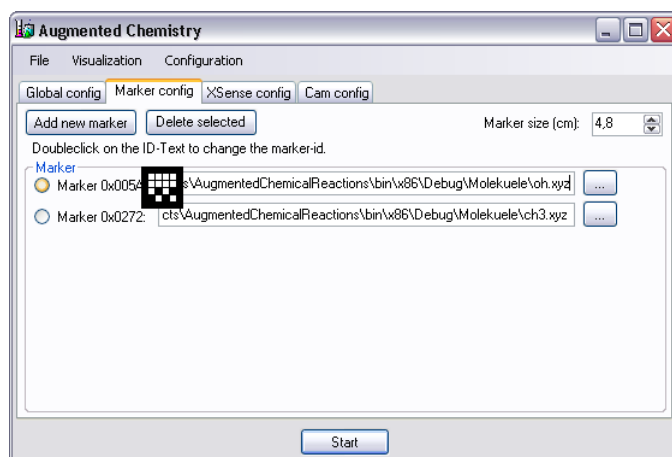


Fig. 4. The user can dynamically assign a molecule description file with a physical marker.

The *Augmented Chemical Reactions* application has a good responsiveness on an average PC. The system uses Windows® and a DirectX® 10 enabled graphics card.

In an user study with high-school students [1], there was mainly positive feedback about the application. The students really liked to interact with the system and would like to use it in class.

III. CONCLUSION

We think that by using a direct manipulation 3D user interface, students can literally grasp the spatial structure. Whereas with mouse and keyboard, there is a mapping of the movements (2D horizontal movement of the mouse on the table results in a rotation of the virtual molecule on the screen). With this mapping, it seems to be not so easy to concentrate on the spatial structure of the virtual molecules. People are used to direct manipulation from their childhood. Consequently this user interface is more natural and supports the learning of the spatial structures.

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