International Journal of Chemical, Materials and Biomolecular Sciences
ISSN: 2415-6620
Vol:3, No:9, 2009

Dynamics in Tangible Chemical Reactions

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***Abstract*—**Spatial understanding and the understanding of dynamic change in the spatial structure of molecules during a reaction is essential for designing new molecules. Knowing the physical processes in the reactions helps to speed up the designing process. To support the designer with the correct representation of the designed molecule as well as showing the dynamic behavior of the whole reacting system is the goal of our application. Our system shows the spatial deformation of the molecules at every time interval by minimizing the energy level of the molecules. The position and orientation of the molecules can be intuitively controlled by manipulating objects of the real world using Augmented Reality techniques. Our approach has the potential to speed up the design of new molecules and help students to understand the chemical processes better.

***Keywords*—**Augmented Chemical Reactions, Augmented Reality, chemistry, education.

I. Introduction

DESIGNING new molecules is a complex and time consuming task requiring spatial understanding. When scientists create a new molecule like a catalyst, they generally first create a model of the desired molecule in 2D which then is transferred to a 3D model in a computer. The 3D computer representation of the molecule is examined to determine if the desired structure can be implemented and provides the desired abilities or if a redesign is necessary. Finally, the molecule is created in the laboratory and tested if it has the desired attributes.

Especially the design, the development and the examination of the spatial 3D structure still bears several issues. Even if the structure of the molecule is represented in 3D, examining the molecule from different perspectives requires the designer to interact with conventional computer input devices. Such devices abstract 3D motion to keys on a keyboard or to the 2D space of a computer mouse. A second issue lies in the changes of the energy setup of the molecule during its development. The spatial structure changes every time a new atom, ligand or radical is added to the existing molecule structure.

To facilitate this development process, we developed a system for visualizing the spatial structure of a molecule and for simulating its dynamic change of the spatial structure while reacting with other molecules or atoms. To achieve this, we have built a 3D visualization tool to present and control models of molecules in an intuitive way. Our system incorporates the paradigm of Augmented Reality (AR), where users can manipulate virtual 3D objects in a simple and intuitive way by moving real 3D objects. The main intention of our system is to show the change of the spatial structure of the molecules during their manipulation. A real-time simulation calculates the attracting and repulsive forces between the reactants of a molecule while these are moved in the interaction space. The motion of tangible placeholders for reactants leads to a dynamic deformation in the structure of the possible molecule product. With this method, scientists can examine design issues at the early stage of molecule design. The opportunity to also change the point of view on the molecule in a 3D interaction space concurrently by using the same tangible handlers extends the capabilities of the system in comparison to conventional approaches that use mice or keyboards for navigation.

Besides the support for molecule design, the presented system also facilitates teaching purposes. Students now can examine different binding principles and 3D structures of molecules from various points of view in an intuitive way. Understanding chemistry depends on understanding the spatial structure of the chemical elements in a molecule. If the spatial structure and dynamic behavior of chemical molecules is conveyed to the students, chemical processes and chemistry per se have the potential to be understood more intuitively.

This paper is structured as follows: We first investigate the issues of computer based molecular modeling in more detail. Then, the paradigm of AR is introduced which is followed by an overview about the application of AR for molecular modeling hitherto. The subsequent chapter illustrates our approach which combines tangible objects with AR and dynamic computation of inter-molecular energy levels. Afterwards, the two fields of application for our system are discussed. The paper then concludes with an overview about the next steps for extension of the system.

II. Issues in Computer-based Chemical Modeling Systems

Conventional computer-based molecular modeling systems bear some inherent drawbacks. The main cause for these drawbacks lies in the nature of the input devices. Computer mice only provide two degrees of freedom while the modeling space has six degrees of freedom, three translational and three

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rotational. Changing the position or orientation of the modeled molecule or the perspective on that model thus is constrained to the two degrees of freedom of the input device. Translation is only possible on a 2D plane and rotations are restricted to two axes. Extensions exist where the state of the controlled axes can be changed, but if even quite fast to learn, the controllability is highly different to 3D motion as we know it from our natural surrounding.

Computer systems for chemical modeling therefore tend to have reduced capabilities for dynamic properties that depend on 3D motion. Such a dynamic property is the examination of a tentative and incomplete molecule structure for possible bonds. Another dynamic property addresses dynamic deformation of a molecule structure when a new atom or radical is to be bound to the structure existing thus far. The subsequent sections investigate these issues in more detail.

A. 3D Visualization and Navigation

For a good perception of the spatial structure, there is the need for an understandable visualization.

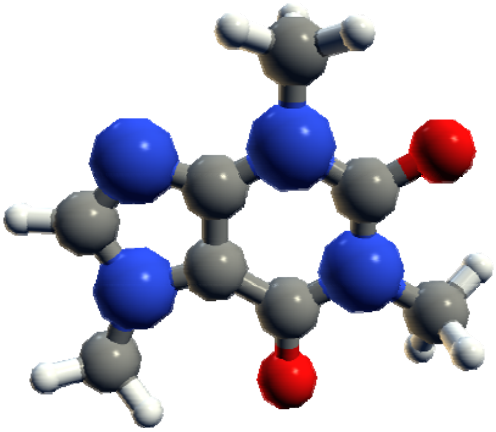


Fig. 1 Ball and Stick Model

A popular representation of molecules is the ball-and-stick model (Fig. 1), which is a 3D or spatial molecular model displaying the structure of chemical compounds, or even biomolecules. In this model, the atoms are represented by spheres around the centre of the atoms. The covalent bond between two atoms is displayed as a cylinder. Double and triple bonds are often represented by two respectively three parallel cylinders between the atoms. The sizes of the atoms cannot be displayed with correct absolute values, but the relation between the atom sizes is correct and uses the “van der Waals radius”. Bond angles and bond lengths reflect the actual relationships from the atomic scale.

Another representation is the so called “space filling” model (Fig. 2), where only spheres with the size of the “van der Waals radius” are drawn. Other visualization strategies can display forces and energy levels between the atoms in a molecular structure.

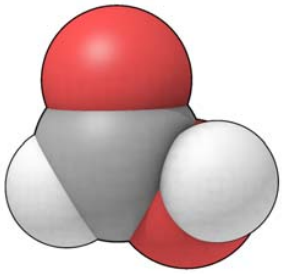


Fig. 2 Space Filling Model

Having different opportunities, the designer of a molecule can switch between different modes to examine the properties of the molecule. The examination process not only requires these different visualization modes but also suitable means of navigation to inspect the molecule from different perspectives. The molecule either must be rotatable, moveable and zoomable, or the user's point of view must provide such properties of motion. Appropriate visualization and the possibility to move in an intuitive way then provide the potential to efficiently investigate molecule structures and dependent physical and chemical properties. For instance, bonding angles can be examined, or accessibility of reactive structures can be inspected.

B. Finding Open Bonds

Design processes for new molecules often take existing reactive structures to compound them together with further atoms into a new, larger molecule. Different principles can be used for such a process: a textual representation can be typed in and then loaded into the 3D visualization or a 3D structure can be loaded to the model existing thus far and bound together. The designer in both cases has to explicitly connect the two open bonds. When the developing molecule structure has several open bonds, the designer has to select one of the open bonds to compound both parts. When working with a textual representation, the designer has to parse the listing manually. When working on the 3D model, the designer has to navigate through the model to find the open bonds. To support the designer in finding these open bonds, there is the need to visualize them in a way to be easily discovered.

C. Dynamicity in the Spatial Structure and Simulation

Dynamic behavior of the spatial structure of molecules while interacting with them, could be important for the understanding of chemical reactions as well as for validating the desired attributes of designed molecules. Every time a new atom or structure is bound to a molecule, its internal structure changes. Incorporating the energetic influence of the new atom, all atoms in the molecule get into another spatial setting. The energy level of the whole molecule thus gets into the lowest possible level.

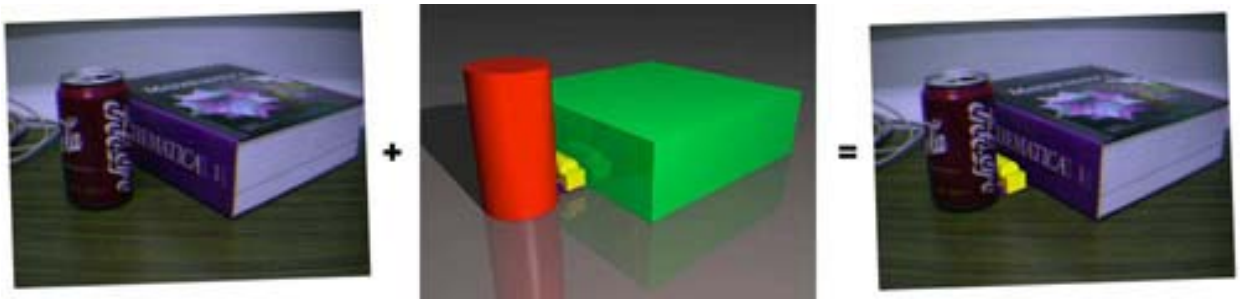


Fig. 3 Basics of Augmented Reality

When designing a molecule, the designer has to check whether the existing structure can accommodate a new group and whether the deformation of the bonding angles keeps the reactive parts of the molecule accessible. Conventional modeling software for chemistry usually computes the new molecule structure at the point in time when a new atom is attached and then renders the new layout on screen. With this principle, the 3D model changes instantly. To determine the structural changes, the designer must memorize the previous setup, has to examine the new structure and has to compare both.

Having a system that shows the deformation already while a new element is approaching could reduce the effort a developer has to invest for building a new structure. In fact, it might not be useful to show how the whole reaction occurs in detail. Instead, a visualization only showing how the molecule structure bends according to the distance of the open bond from the new atom might be useful. Such visualization could have the potential to facilitate the understanding of the energetic effects of chemical reactions.

A developer of a molecule could move a new atom towards the molecule existing thus far. The structure then bends smoothly according to the attracting and repulsive forces. The developer can follow the way of each atom in the molecule as it smoothly moves away. This could show, especially in the case of larger molecules, why some reactions are not possible. For example after binding a new atom, an initially free area would shrink in a way that a further, larger structure would not fit into that area.

III. Augmented Reality

Augmented Reality 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.

Fig. 3 shows the basic concept of Augmented Reality. In addition to the real world with its real 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 loosing the 3D connection to the virtual object.

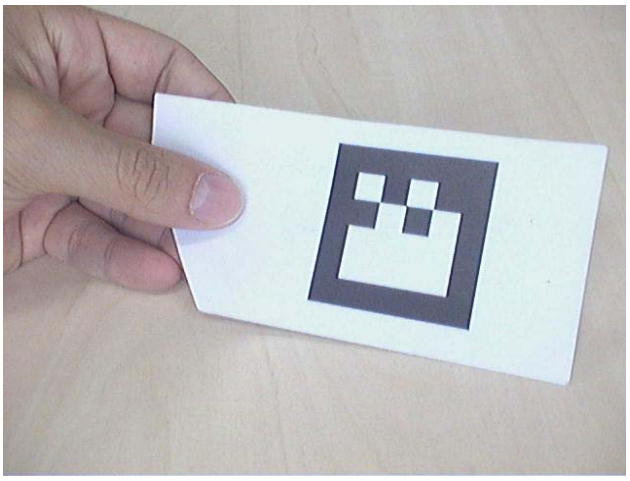
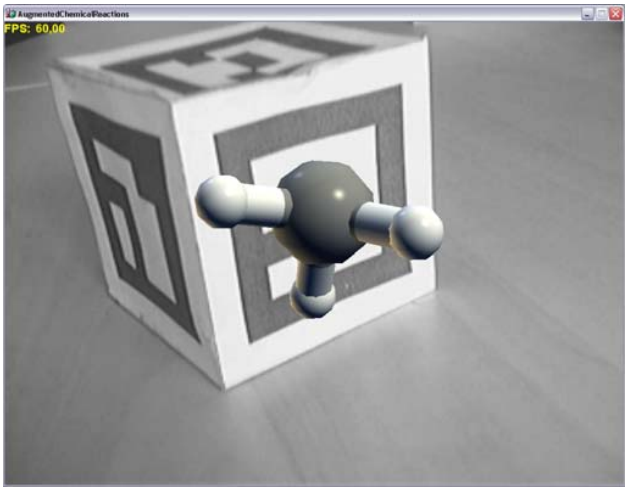
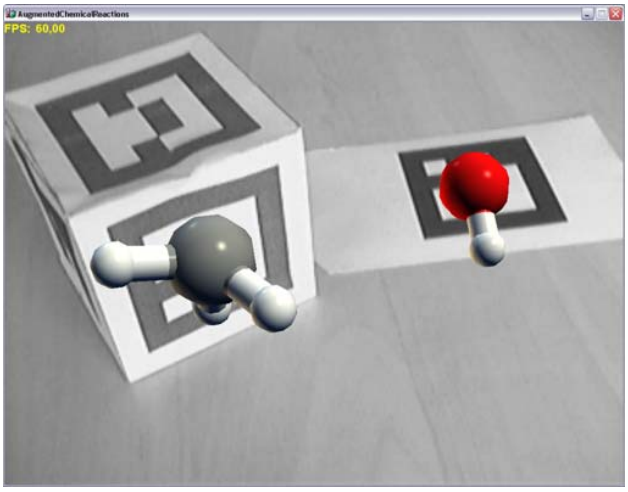


Fig. 4 Example of a marker

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 (Fig. 4). The position and rotation of the marker relative to the webcam is calculated with computer vision algorithms. Two main systems are AR-ToolKit [1] and UbiTrack [2]. This data is then passed to the Augmented Chemical Reactions application that uses this to calculate and control the molecules.



(a) Marker with a molecule rendered on it



(b) Multiple markers each with molecules rendered on top

Fig. 5 Augmented markers

IV. Related Work

There are few supporting tools in chemistry that use Augmented Reality. To increase the learning effectiveness in chemistry education, Morten Fjeld et al. built Augmented Chemistry [3], an application that uses a tangible user interface for education of organic chemistry. They compared learning effectiveness and user acceptance of Augmented Chemistry (AC) versus the more traditional ball-and-stick model. Results in learning effectiveness were almost the same for both learning environments. User preference and rankings, using NASA-TLX [4] and SUMI [5], 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.

Suzanne Weghorst described in an report [6] the progress to date on an at that time ongoing joint research project between the HIT Lab at the University of Washington and the Molecular Graphics Lab at The Scripps Research Institute (TSRI). The goals of this research are to develop and evaluate novel interface tools for teaching and conducting research in the field of molecular biology. These interface tools are integrated within TSRI's python-based molecular viewer (called PMV). Specifically, they are enhancing PMVgenerated 3D physical models of complex molecules with mixed reality graphics, sound, voice interaction, and haptics. Lessons developed using these tools were tested in both high school and college level classrooms, and alternative approaches have been evaluated.

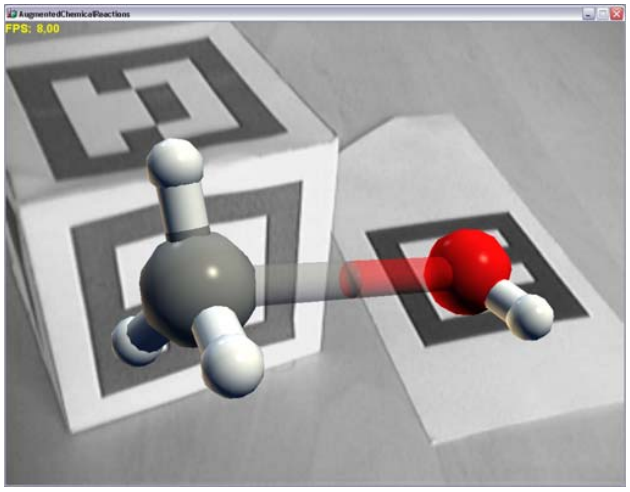
This system is intended to directly create physical 3D models of molecules, which are overlaid with additional information such as electrostatic fields.

Recent studies have been made by Eliana Medina et al. with static molecules to help students learn biochemistry [7].

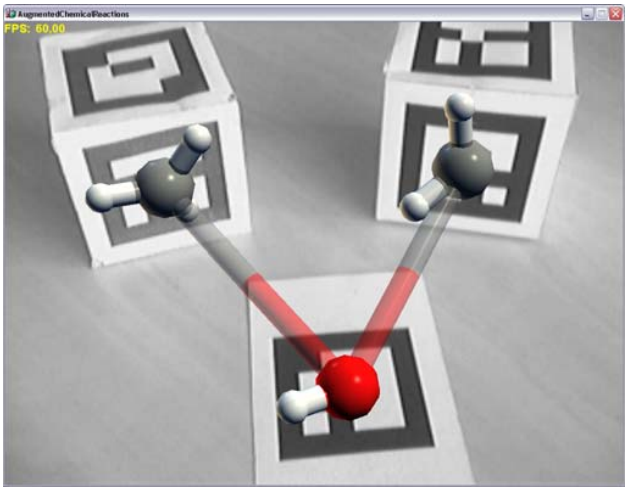
Further related work was done by Morten Fjeld et al. [8], [9] and Hannes Kaufmann et al. [10] where only static molecule structures can be inspected and built with instantaneous changes.

V. Augmented Chemical Reactions

The process of designing new molecules, as for example catalysts, is a time consuming task. While designing those catalysts, there is a strong need for taking the dynamic change of the bond angles into account. Unwanted deformations of the spatial structure of the molecules while trying to react with the catalyst could prevent the reaction. To support chemists in the process of designing and validating catalysts, we have designed and implemented Augmented Chemical Reactions, a visualization program for chemical molecules and chemical reactions. With this tool, it is possible to inspect molecules in an intuitive way as well as showing the dynamic behavior of the molecules while interacting with them. Chemists only have to create the desired molecule structures in their preferred application (for example MOLDEN [11]) and load the generated molecule description file into the Augmented Chemical Reactions program. Only a cheap webcam and markers (Fig. [4]) are required, which are easily self made by printing a special pattern on a piece of paper. To achieve an intuitive interaction with the molecules, the visualization of the molecules can be assigned to different markers (Fig. [4] When holding this marker in the field of view of the webcam, the model of the molecule is rendered on top of the marker in the webcam picture on the screen (Fig. 5(a)).



(a) One possible bond between two atoms



(b) More possible bonds

Fig. 6 Molecules reacting with each other

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 was 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 to additional molecules (Fig. 5(b)), allows visualizing and interacting with more molecules at the same time. With different 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 smaller than a given value (here 5Å) and the atoms have the ability to bind, a possible bond is drawn, represented by a transparent cylinder connecting those two atoms. The molecules are starting to deform due to the forces between the molecules (Fig. 6(a)). The dynamic transformation of the molecules is done by an optimizer out of the TINKER package [12], that optimizes the structure of a molecule by minimizing the energy of the molecule. Simulating only one molecule allows the inspection of the molecule in its right spatial confirmation. When interacting with more than one molecule not bond to each other at the same time, the optimization program would take the whole system into account. As a result, the molecules would be separated in the simulation, due to the repulsive forces between the molecules. To prevent this behavior and give the feeling of holding the molecules in the hands of the user, there is the need to freeze the distance and position of the centre atoms of the molecules to the distance and position of the markers. This leads to a deformation of the spatial structure of the molecules because of the attracting and repulsive forces. This interaction is the intuitive correspondence to holding ball and stick models of atoms at their centre atoms, allowing to deform the surrounding atoms.

The simulation calculates in real-time the optimized version of the whole system with the fixed distance of the centre atoms, defined by the distance of the markers.

Fig. 6(b) shows additional transparent cylinders drawn between the molecules, when there are more potential bonds. The designer must not only be able to see the next possible bond at a time, but also which other possible bonds are available. Possible bonds could be visualized in different ways. Transparent cylinders between the linking atoms, as well as dashed lines or curves are possible. When there is more than one possibility, where molecules can react, multiple possible bonds have to be displayed to the users. The selection of one particular possible bond out of these can be supported by highlighting the possible bond that has the strongest binding forces.

VI. Fields of Application

A. New Opportunities for Science

For scientists the process of designing new molecules, such as new catalysts, is currently a time consuming task. When they design a new catalyst for a special reaction, they first have to develop this possible molecule, and create it in the laboratory. It will take some days to generate the desired molecule in a complex series of reactions. 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. It also shows the dynamic behavior of the molecule models while their distance falls below a certain value. This allows a better understanding of the chemical processes than in a static examination. If the designed catalyst does not fulfil the criteria, the molecule can be modified without much loss of time due to creating it in the laboratory.

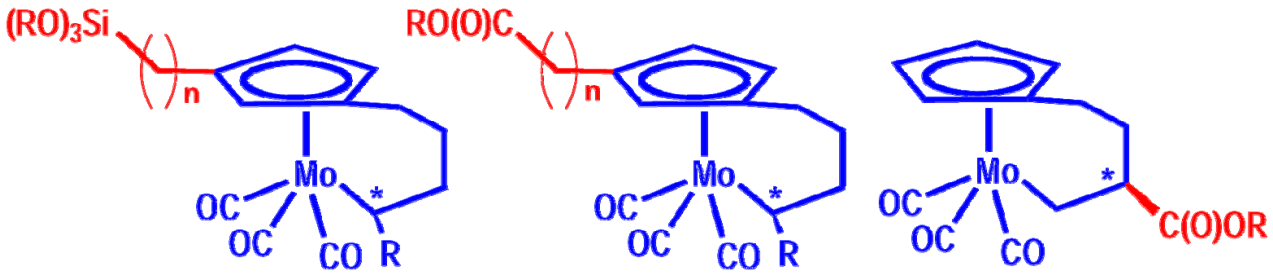


Fig. 7 Organomolybdenum complexes

One actual application of Augmented Chemical Reactions is the design of a catalyst to control the chirality of the products of a catalysis. In this special case Organomolybdenum complexes as seen in figure 7, will be both immobilized and attached to chiral ligands in order to enable easy catalyst/product separation and chiral catalysis. In this 2D representation of the chemical formula for the catalyst, it is hard to see the exact spatial configuration of that molecule. As a result of this, the designed molecules could not have the desired chiral attribute. In a catalysis with this molecule, the reactants should only have one possible place where they react, due to the chiral attribute of the catalyst. The chiral attribute is set up by placing a ligand at a special place on the catalyst to block a reaction at an unwanted position of the catalyst. When this ligand is not at the desired position due to lack of the spatial knowledge, unwanted products could be roduced in the catalysis. Even when the catalyst itself has the correct spatial structure in a static observation, the spatial structure can change in an undesired way when the reactants approach the catalyst because of the attractive and repulsive forces. In such case the desired chiral attribute is not given anymore.

When inspecting the designed catalyst with Augmented Chemical Reactions, the spatial structure of the catalyst, especially of the ligand defining the chirality can be validated. This reduces unnecessary and time-consuming creations and tests of the catalyst in the laboratory.

B. New Opportunities for Teaching

This application also offers new opportunities for teaching and education, because 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 one 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 change in the spatial structure 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. Students 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 as shown in figure 5 and 6) 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.

VII. Future Work

Future work now has to determine, which gestures and user input methods to interact with the molecules are easy and intuitively to use. If it is for example necessary to use more than two molecules at the same time with more than two markers, it will be difficult to control the three objects 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 bond is displayed to the user. The selection of the desired bond could be visualized by altering the color or transparency of the possible bonds in respect to the actual energy of this bond. So the possible bond that has the strongest binding forces could be visualized with the lowest transparency.

VIII. Conclusion

Augmented Chemical Reactions could increase the understanding of chemical processes as well as helping to design new molecules with certain attributes, because it shows the spatial relations and dynamic deformation between molecules and their resulting reaction. 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. For educational purposes, Augmented Chemical Reactions also has the potential of increasing the learning effectiveness of chemistry.

References

[1] H. Kato and M. Billinghurst, "Marker tracking and HMD calibration for a video-based augmented reality conferencing system," in *Augmented Reality, 1999. (IWAR '99) Proceedings. 2nd IEEE and ACM International Workshop on*, 1999, pp. 85–94.

[2] M. Huber, D. Pustka, P. Keitler, F. Echtler, and G. Klinker, "A System Architecture for Ubiquitous Tracking Environments," *in Proceedings of the 6th International Symposium on Mixed and Augmented Reality (ISMAR)*, Nov. 2007.

[3] M. Fjeld, J. Fredriksson, M. Ejdestig, F. Duca, K. Botschi, B. Voegtli, and P. Juchli, "Tangible user interface for chemistry education: comparative evaluation and re-design," in *CHI '07: Proceedings of the SIGCHI conference on Human factors in computing systems.* New York, NY, USA: ACM, 2007, pp. 805–808.

[4] NASA, "NASA TLX: Task Load Index," http://humansystems.arc.nasa.gov/groups/TLX/, Last accessed, May 2009.

[5] University College Cork, "Software Usability Measurement Inventory," http://sumi.ucc.ie/, Last accessed, May 2009.

[6] S. Weghorst, "Augmenting Tangible Molecular Models," in *Proceedings of International Conference on Artificial Reality and Telexistence*, Tokyo, Japan: IEEE, 2003, pp. 1–6.

[7] E. Medina, Y. Chen, and S. Weghorst, "Understanding biochemistry with Augmented Reality," in *C. Montgomerie & J. Seale (Eds.) Proceedings of World Conference on Educational Multimedia, Hypermedia and Telecommunications 2007*, Chesapeake, VA: AACE, 2007, pp. 4235–4239.

[8] M. Fjeld, P. Juchli, and B. Voegtli, "Chemistry Education: A Tangible Interaction Approach," in *Proceedings of IFIP INTERACT03: Human-Computer Interaction*. IFIP Technical Committee No 13 on Human-Computer Interaction, 2003, p. 287.

[9] M. Fjeld and B. M. Voegtli, "Augmented Chemistry: An Interactive Educational Workbench," in *ISMAR '02: Proceedings of the 1st International Symposium on Mixed and Augmented Reality*. Washington, DC, USA: IEEE Computer Society, 2002, p. 259.

[10] H. Kaufmann and A. D¨unser, "Summary of Usability Evaluations of an Educational Augmented Reality Application," in *HCI (14)*, 2007, pp. 660–669.

[11] G.Schaftenaar and J. Noordik, "MOLDEN a pre- and post processing program of molecular and electronic structure," http://www.cmbi.ru.nl/molden/, Last accessed, May 2009.

[12] N. S. Foundation and U. S. N. I. of Health, "TINKER - Software Tools for Molecular Design," http://dasher.wustl.edu/tinker/, Last accessed, May 2009.