

Augmented Chemical Reactions

Small molecules with a large impact

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Abstract

Modeling of molecular catalysts in chemistry is still a time consuming process. Where chemists design new catalysts in 2D on a screen or a paper, for making special molecules with a defined chirality, Augmented Chemistry provides an efficient way for designing and interacting with the molecules. This helps to understand the spatial relations between catalyst and reacting molecules and accelerates the process of creating a functioning catalyst.

Also for students it is very informative to see what molecules are, and how they can behave and react in a 3D environment with other molecules.

The proposed demo will show the usage of that system with a sample set of two reacting molecules.

Keywords: Augmented Reality, Augmented Chemistry, Tangible Chemical Reactions.

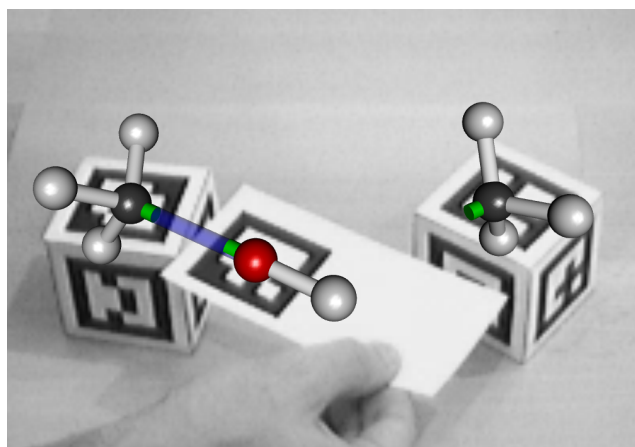


Figure 1. Demonstration of a possible bound

1 Introduction

When creating new chemical products, for example for the pharmaceutical industry, it is very important to create only the desired product in a reaction. This is not always given

by default. Many reactions create more than one product due to the fact of chirality. Therefore catalysts have to be developed very carefully.

State-of-the-art Such development is done in 2D on a computer monitor or even on a piece of paper. The reaction is then tested in the laboratory. Up on failure, the catalyst has to be redesigned and the process starts over again.

Augmented Chemistry Augmented Chemistry can help to speed up the process of designing a working catalyst. Instead of processing the time consuming reaction in the laboratory, the designed catalyst can be visualized and inspected in the 3D environment in front of the chemist. In this environment, the handling of a 3D object with tangible markers is very intuitive and spatial relations as well as the dynamic behaviour between the catalyst and the reacting molecules can be observed, while the reaction takes place. In this state the catalyst can be redesigned without having spent the time for a real reaction in the laboratory.

Education The tangible information given by this system is very useful for students learning chemistry or even professional chemists. Here they can understand how molecules, with a given empirical formula, look in the 3D environment. This will help students in their process of learning and understanding the spatial structure and dynamic behavior of molecules and chemical reactions. For example the visualization, that molecules have dynamic rather than fixed bindings helps users to realize, why a chemical reaction might not succeed even though the empirical formula would allow it.

2 Demo Description

The goal of this demo is to show how quickly and easily it is to build up an environment that can be used to visualize and interact with the molecules.



Figure 2. equipment examples

Viewers will have the opportunity to test and interact with the system.

3 List of Equipment

- 1 laptop running Augmented Chemistry demo software
- 1 webcam
- several markers

4 Space Requirements

The demo requires about $1 \times 2m^2$ of space with a table. Ideal would be some space next to the table to put up a poster. There should be a power outlet for the laptop.

5 Videos

Videos of this demo are available on the project page:

[http://ar.in.tum.de/Chair/
ProjectChemistry](http://ar.in.tum.de/Chair/ProjectChemistry)

or separately (Viewed with a FlashVideo-Player):

[http://campar.in.tum.de/files/movies/
flash_movies/ProjectChemistry.flv](http://campar.in.tum.de/files/movies/flash_movies/ProjectChemistry.flv)

[http://campar.in.tum.de/files/movies/
flash_movies/ProjectChemistry2.flv](http://campar.in.tum.de/files/movies/flash_movies/ProjectChemistry2.flv)

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