

Augmented Chemical Reactions

Patrick Maier, Markus Tönnis, Prof. Gudrun Klinker
Fachgebiet Augmented Reality
Department of Computer Science
Technische Universität München

Overview

- 1. Augmented Reality**
- 2. Augmented Chemical Reactions**
- 3. Help in Education / Science**
- 4. Dynamic Spatial Deformation**
- 5. Future Work**

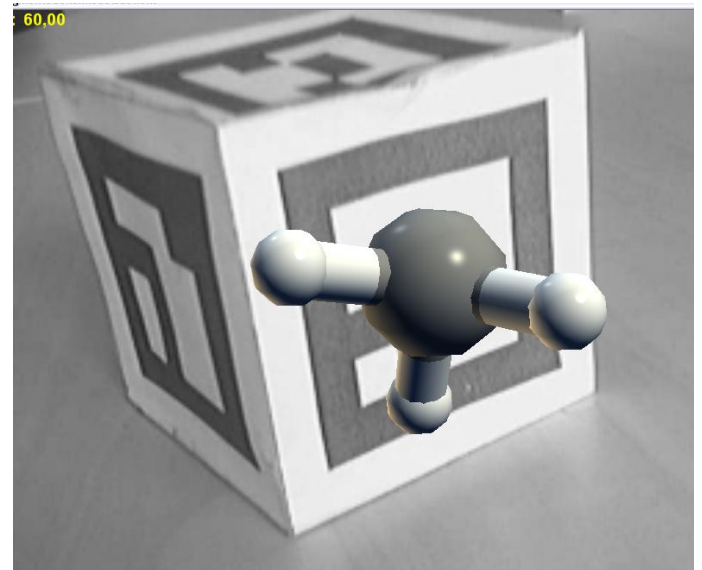
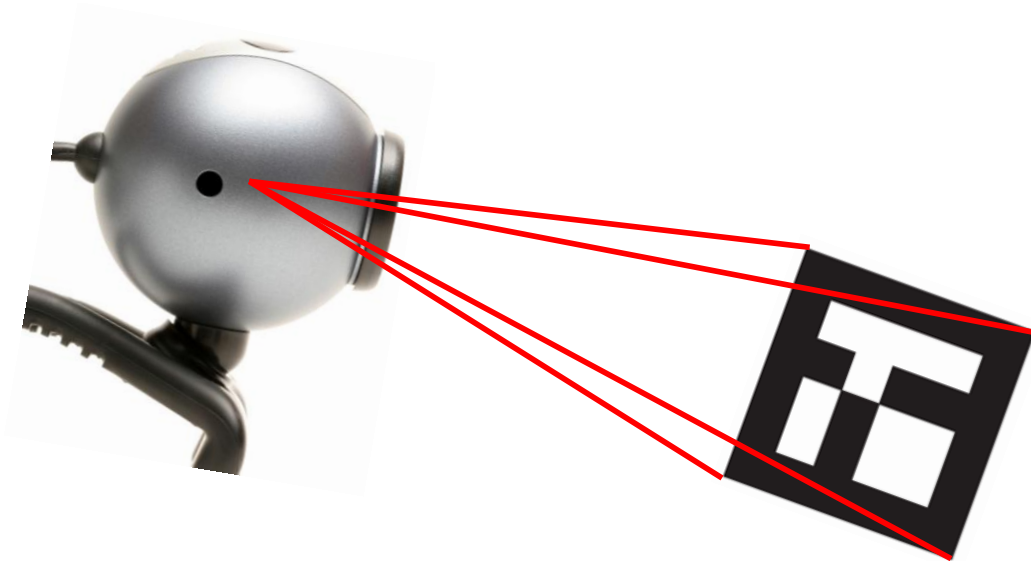
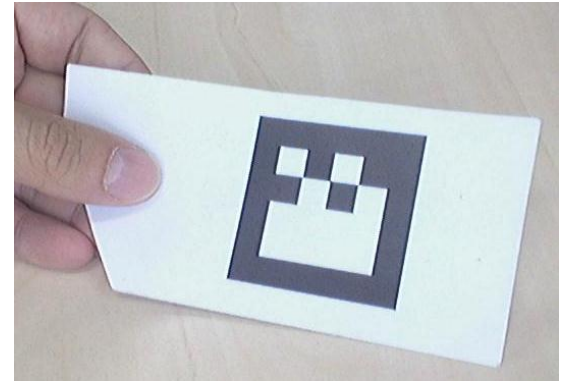
Augmented Reality Technique

- Combines Reality + Virtual Objects
- Interactive in real-time
- Registered in 3 Dimensions



Augmented Reality - Technology

- Manipulation of real objects (markers)
- Webcam takes picture of the markers
- Calculating the position and orientation of the markers
- Augment the picture with virtual objects



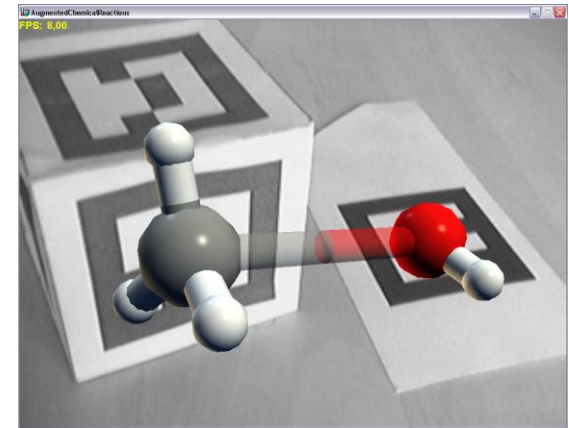
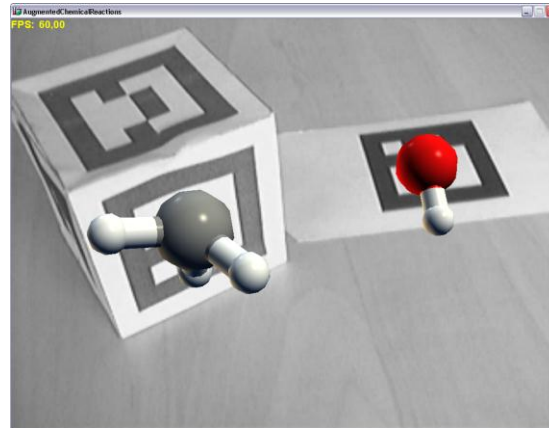
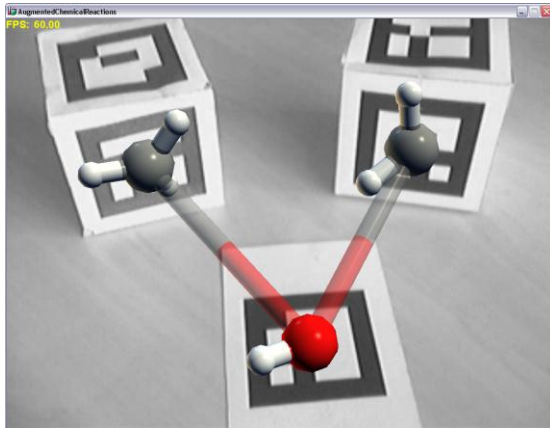
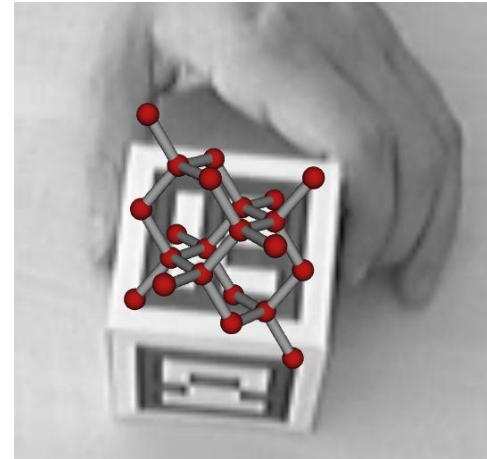
Augmented Chemical Reactions

Augmented Reality for Chemistry

- Help to understand
- Help to design molecules

Because

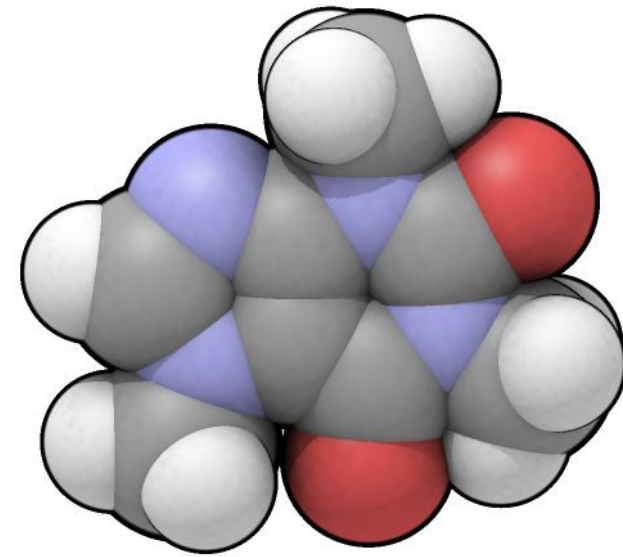
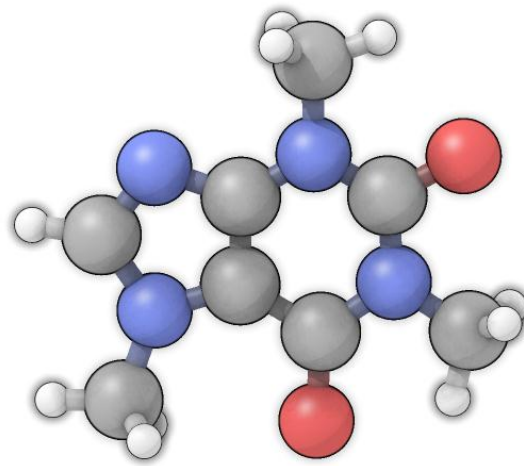
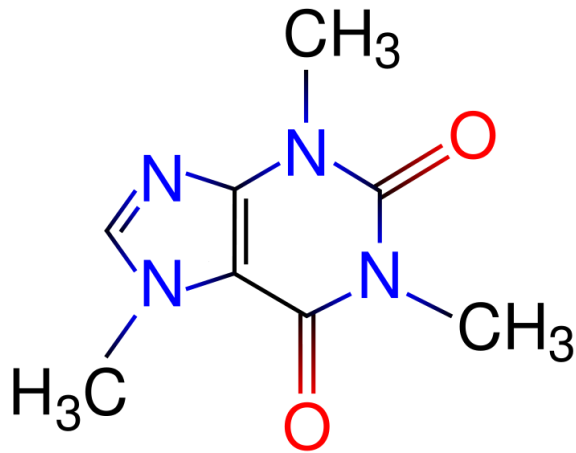
- Inspect molecules intuitively
- Show the dynamics
- Tangible molecules/reactions



Help to understand chemistry

Help to understand:

- Educational help
- Improve 3D understanding of molecules
- Inspect molecules in an intuitive way

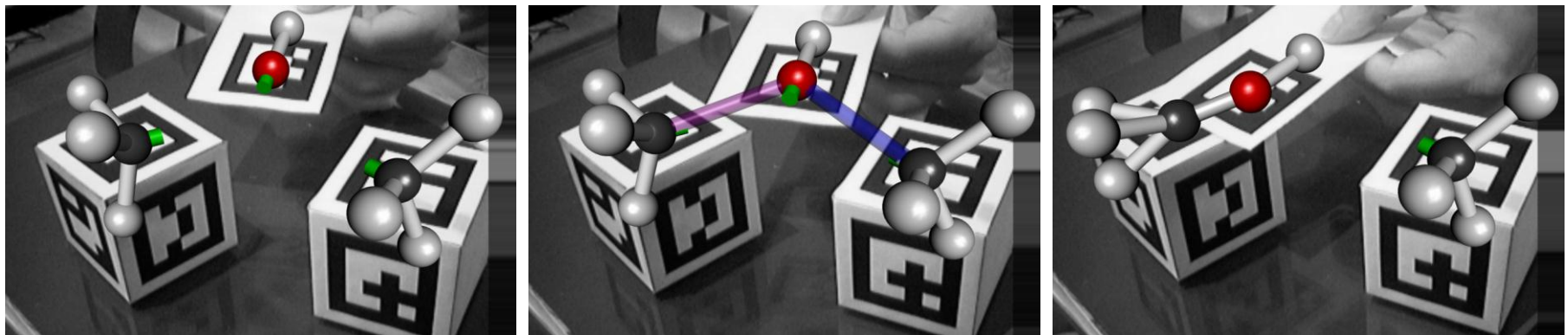


Caffeine: $C_8H_{10}N_4O_2$

Dynamic spatial deformation

New in this topic:

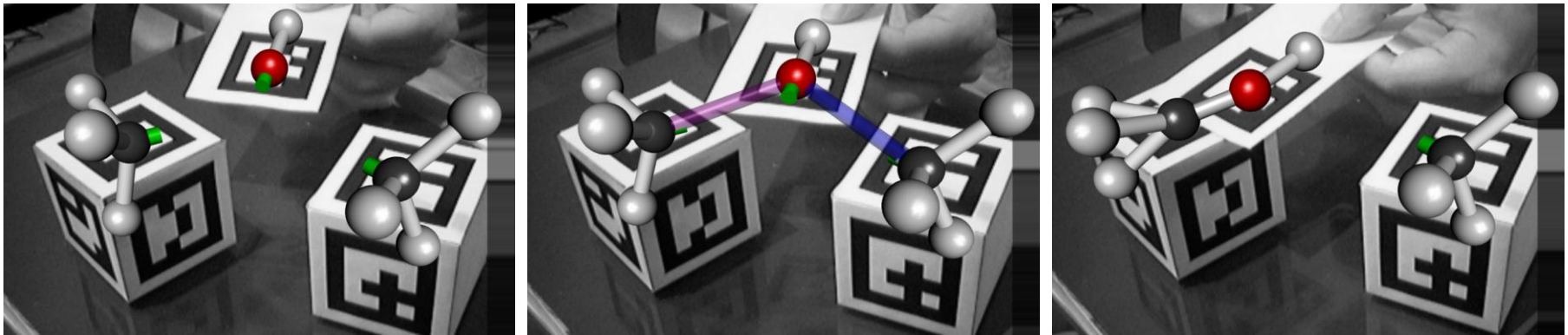
- Dynamic behavior between molecules
- Real-time optimization of the molecules while controlling the position and orientation
- Show possible bonds



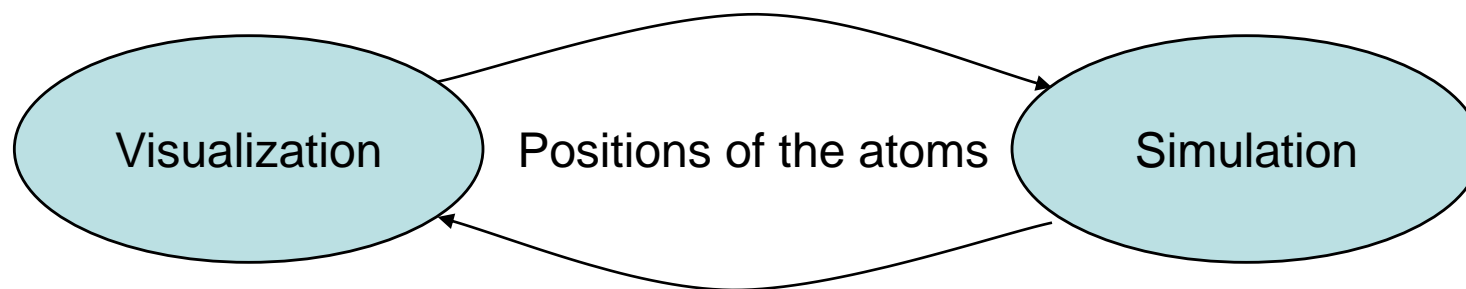
Dynamic spatial deformation

Simulation /Optimization package: TINKER

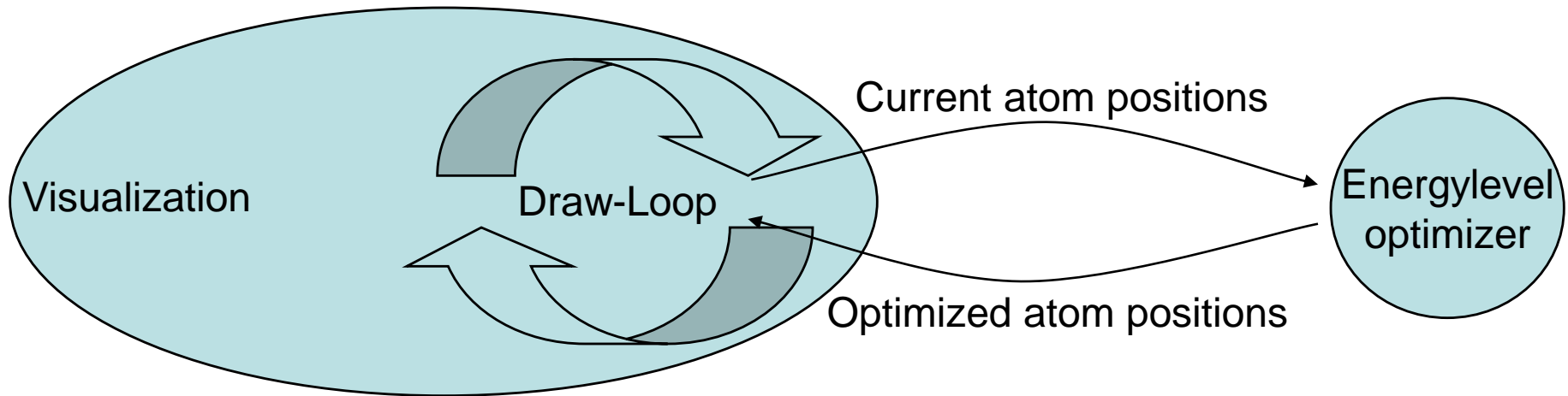
- Fixate one atom of each molecule to the marker.
- Optimize every time interval.
(Minimize the energy level of the molecules)
- Show the results.



Dynamic spatial deformation



Dynamic spatial deformation



Dynamic spatial deformation

Process of optimizing the molecule structures:

- One molecule:
 - Just pass the atom positions and bonds
- Multiple molecules:
 - Passing just the atom positions is not sufficient → molecules would drift away
 - Fixate one atom per molecule to a given position (Marker position)
 - If the molecules are near enough → connect the molecules and handle as one molecule in the simulation

System interaction

Problem of two handed interaction with the system:

- How to connect two molecules permanently?
 - Gesture to connect the molecules.
- To which marker do we want the connected molecules to stick to?
 - Gesture to select a marker.

Augmented Chemical Reactions – Future Work

- New user interface methods
- New gestures for interaction
- Stereoscopic display (HMD)

Thank You

Used Technique

- **Programming language: C#**
 - Faster development of window applications
 - Large set of helper-classes (.NET framework)
 - (Tried C++ without .net framework, too much work)
- **Tracking: UbiTrack-Library (with wrapper for managed C#)**
 - Supports large set of input devices (sensors)
 - Combination of several devices (sensor fusion)
 - Highly configurable (UTQL)
- **Visualization: Microsoft XNA**
 - Uses DirectX
 - Easy to use
 - Natively in C#
 - Portable to Xbox
 - (Tried C++ OpenSceneGraph. Wrapper for C# was too slow)
- **Simulation: TINKER**
 - Free molecule optimizer application