

Dynamics in Tangible Chemical Reactions

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Overview

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

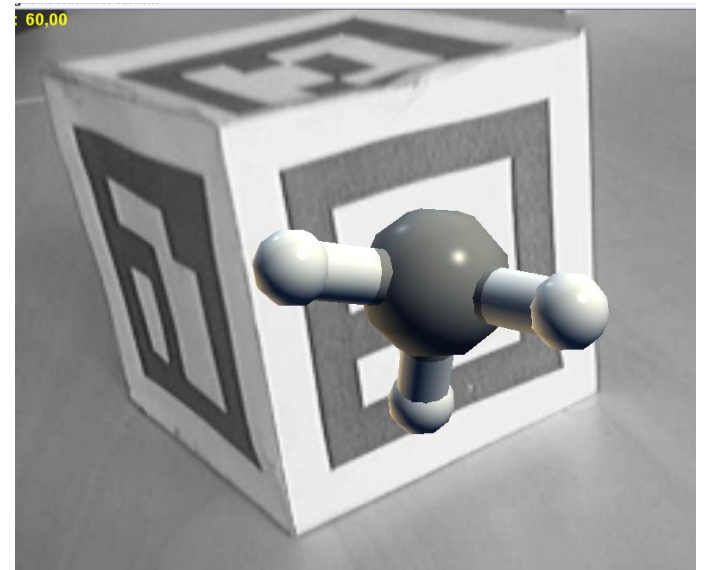
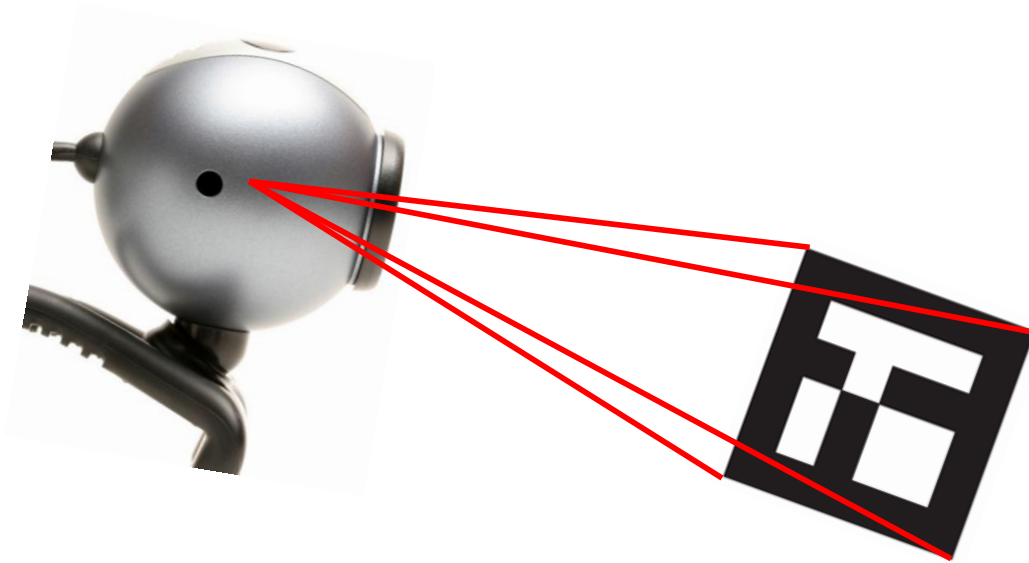
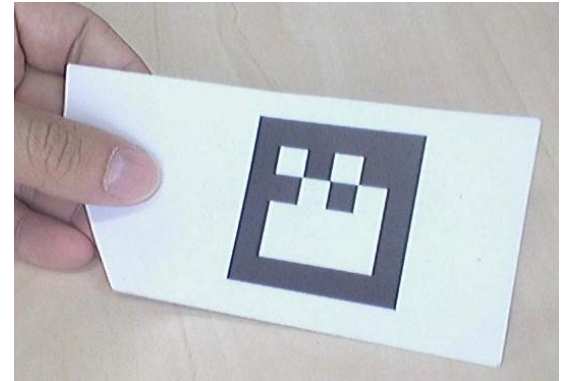
Augmented Reality Technique

- 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



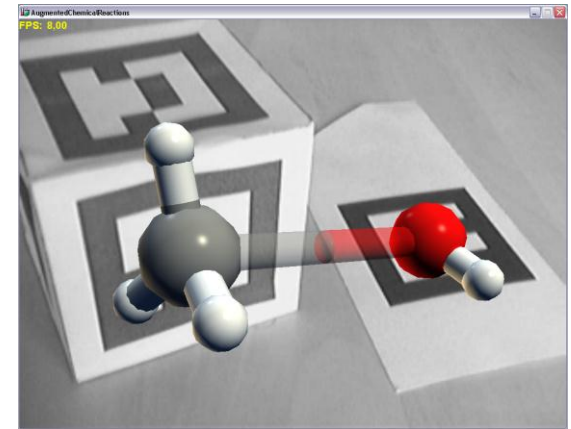
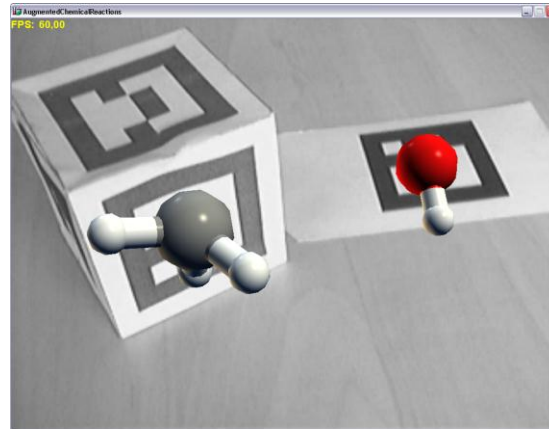
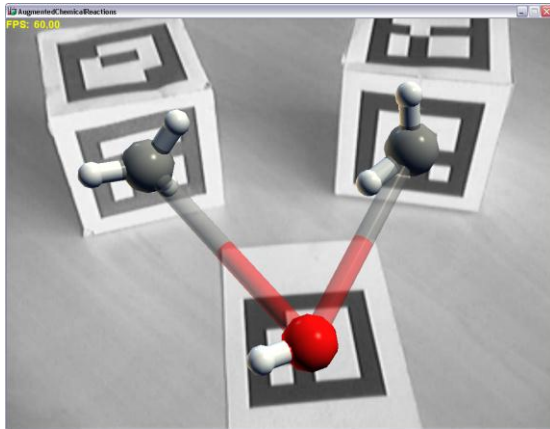
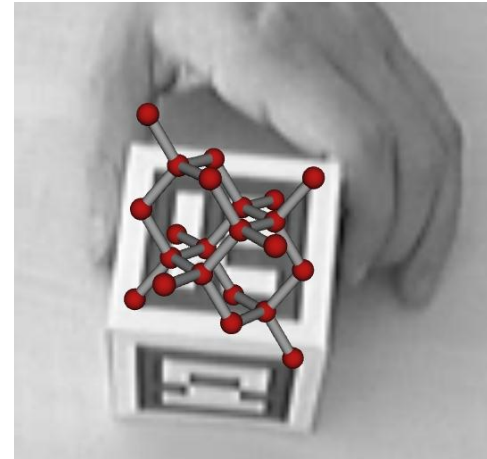
Augmented Chemical Reactions

Augmented Reality for Chemistry

- Help to understand
- Help to design molecules

Because

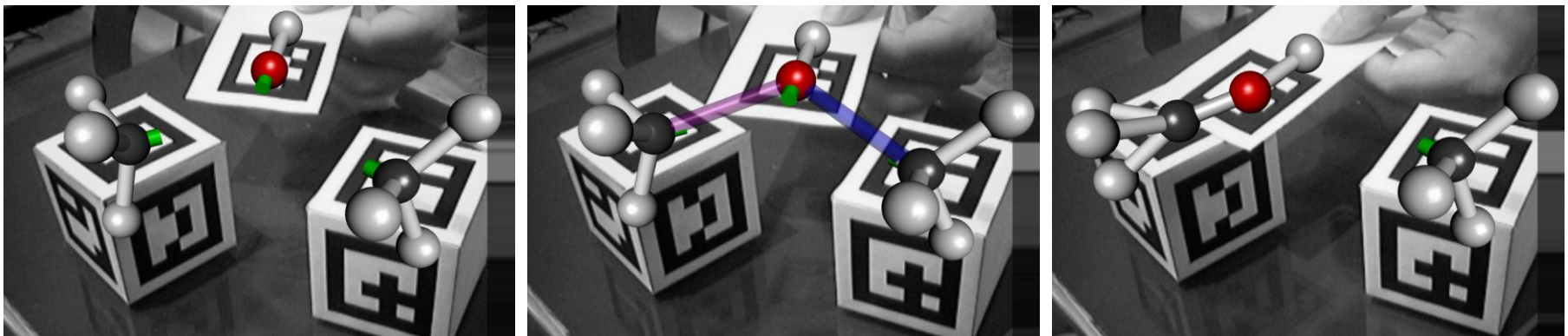
- Inspect molecules intuitively
- Show the dynamics
- Tangible molecules/reactions



Dynamic spatial deformation

New in this topic:

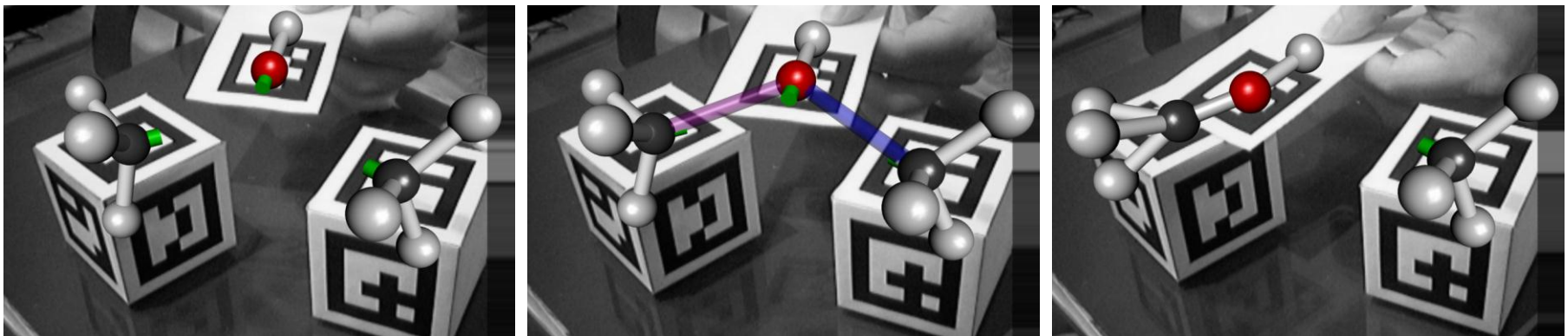
- Dynamic behavior between molecules
- Real-time optimization of the molecules while controlling the position and orientation
- Show possible bonds



Dynamic spatial deformation

Simulation / Optimization package: TINKER

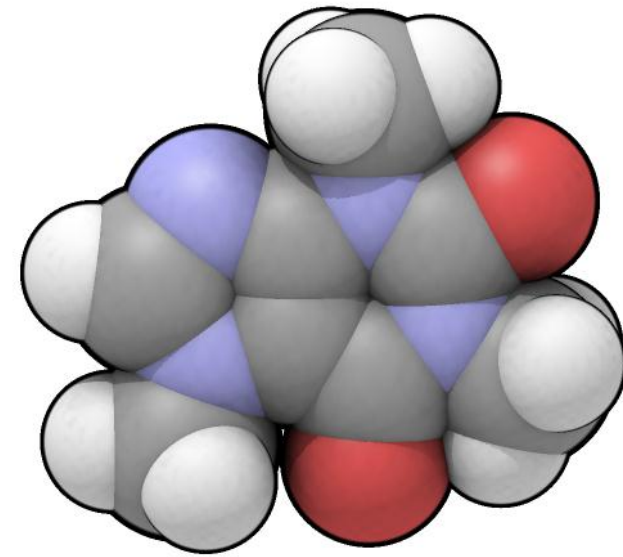
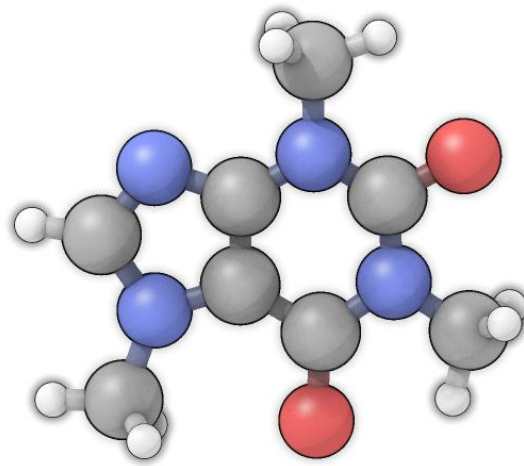
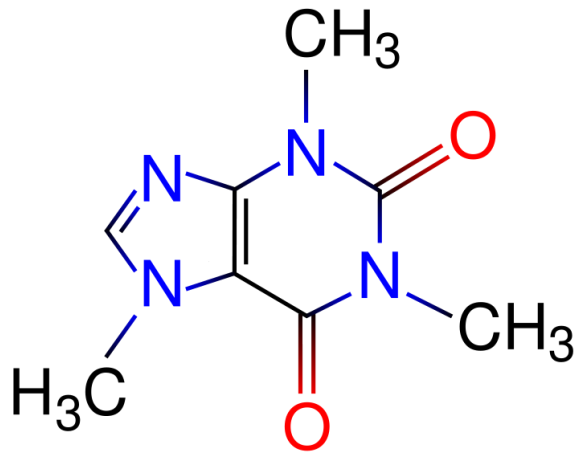
- Fixate one atom of each molecule to the marker.
- Optimize every time interval.
(Minimize the energy level of the molecules)
- Show the results.



Help to understand chemistry

Help to understand:

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



Caffeine: $C_8H_{10}N_4O_2$

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