Augmented Chemical Reactions

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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

Visualization \rightarrow \text{Positions of the atoms} \rightarrow \text{Simulation}
Dynamic spatial deformation

- Visualization
- Draw-Loop
- Current atom positions
- Optimized atom positions
- Energy level optimizer

Augmented Chemical Reactions
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