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Augmented Chemistry: An Interactive Educational Workbench

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Abstract
This system paper reports on some of the advantages tangible interaction can bring to chemistry education. The paper describes the realisation of an in-house designed Tangible User Interface (TUI) called Augmented Chemistry (AC). A set of interactive tools work within this system. Using these tools, elements can be chosen from a booklet menu and composed into 3D molecular models. The tools indicate one way towards realising a seamless integration of the physical and digital realms. Since many tools can be used concurrently, single and multiple users can interact with the system at a time. To use the system in an educational context, it was extended into an educational workbench drawing on haptic and aural augmentation. The design and implementation of the AC system required contributions from optics, mathematics, molecular chemistry, software engineering, and 3D programming, making it a truly interdisciplinary project. Future challenges lie in user acceptance, educational effect, and further system development.

Keywords
AR educational application, chemistry education, display hardware, haptic and aural augmentation, tangible user interface (TUI)

3D INTERACTION IN AR WORKBENCHES
While some TUIs offer planar interaction, such as Tangible Bricks [4], other systems offer 3D interaction, such as Cubes [3][6]. Wireless tracking of interaction handles may be either optical [3][4][5][6] or electromagnetic [7]. This paper reports on an in-house designed TUI performing 3D optical tracking of an interaction cube. Such systems can benefit 3D interaction by offering a more direct form of interaction coming closer to the use of physical artefacts and tools. This offers users a more natural use of hand and body movements. Such movements may hence be integrated into the interaction with digital information, thereby supporting a fluent handling of 3D models [5].

INTERACTIVE FORM
Based on a Tangible User Interface (TUI), the application Augmented Chemistry (AC) was designed. The AC system is a workbench offering its users to see and to interact with 3D molecular models in an 'intuitive' and 'direct' way. The system also offers tools to build composite molecular models. Following a common use of AR Toolkit [2], a cube with printed patterns is connected to an animated 3D model and both are seen in a mirror image. Using a specialized select- and rotate-tools, single atoms can be picked up, positioned, and composed into complete molecules. Chemical rules can be formulated and integrated into the application, thus enabling the construction of basic structures as appearing in the nature, for instance water.

SYSTEM SETUP
Augmented Chemistry (AC) is a workbench consisting of a table and a rear-projection screen (Fig. 1). The screen is based on acrylic glass from Lumin™. It is particularly well suited for rear-projection and also works well under daylight conditions. Right below the screen sits a camera recording user interaction taking place upon and above the tabletop. The screen displays what this camera sees. Such a display is meant to give the user the feeling of a mirror. This mirror image is then enriched with a virtual environment. Users interact with models in this virtual environment using a booklet, a cube, a platform, and a so-called Gripper. Each page in the booklet is used to identify an element of the periodic table. The booklet, the platform, and the Gripper each carry a pattern; the cube carries six patterns − one per page. A 3D model augments the mirror image of a booklet page, a platform, a cube, or a Gripper (Fig. 2). Hence, users can select, position, rotate, compose, and deselect 3D models, thereby affecting the virtual environment.

Figure 1. System set-up with a typical situation of use: charging the Gripper with an element from the booklet (left). The platform (right) holds an unsaturated atom, with which a binding with the charged atom may be triggered.

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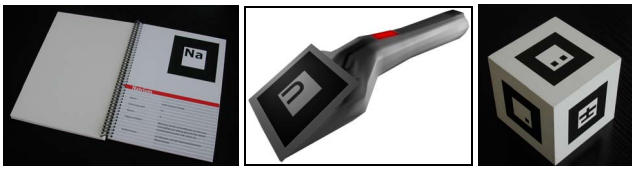
INTERACTIVE TOOLS

Bringing together two elements triggers the composition of a molecular model. This operation requires the use of both hands, called bimanual interaction [1]. The booklet shows elements by a printed picture and a name. One hand browses the booklet, offering one element per page (Fig. 2a). Using a so-called Gripper (Fig. 2b), users can pick up elements from the booklet. The term gripper stems from robotics and implies a tool with jaws. Instead of jaws, this Gripper has a button used to bind an atom to the molecular model. First, bringing the Gripper into a small perimeter around the element in the booklet charges the Gripper with that element. Second, the Gripper is positioned next to the platform. The platform holds a molecule. With the rotation of a cube (Fig. 2c), operated by the second hand, users can determine where and how (single- double- or triple-binding) the element shall connect to the molecule.



a b c

Figure 2. a) Booklet offering one element per page – here Na – sodium. Each element is represented by a pattern. b) Gripper with a button (red) and a pattern. c) Cube with one distinct pattern for each surface.

AURAL AUGMENTATION

We set out to offer an audio feedback suited to each molecule constructed. Such feedback can be considered as aural augmentation of the molecular models. During the constructions of a molecule, different states trigger visual and audio events, being:

- When a molecule is saturated (state), i.e. no more bindings can take place, an acoustic signal is triggered (event). This tells the user that he or she can move on to construct the next molecule.
- When a molecule belongs to the predefined list (state), the user is offered additional spoken information about the molecule (e.g. „water covers 75% of the surface of the earth …") (event).

COMPOSITE MODELS

In pursuing the issue of composite molecular models, some challenges have been met. On the one hand, these are raised by so-called isomerism, describing molecules of same sum formula but of different constitution (that is bindings or connections). Stereoisomeres are molecules of the same constitution but different geometries (diastereomeres) or topographies (enantiomeres). The AC system cannot distinguish stereoisomeres and no general way to compare such complex structures have come to the authors' knowledge. On the other hand, the educational scope of the AC application makes it crucial to keep track of user actions. Such tracking enables both an identification of new composite molecular models and offers appropriate system feedback to its users. Altogether, this represents a challenge to chemistry education and to the AC system design.

VISUAL REPRESENTATION

To represent molecular models graphically, the AC system employs a well-known principle, namely the ball-stick model. In the booklet, working as an interactive menu, the valence of an atom can be seen. Visualizing the number of electrons in the valence shell shows the valence. Firstly, the visual representation of atoms is different from that of the molecules. Secondly, atoms are not only shown as coloured balls. Rather, they are visualized with a clearly visible nucleus and the outermost valence shell. This representation of atoms is in accordance with the model of Bohr.

FUTURE PERSPECTIVES

Firstly, the extension of the AC system functionality towards offering a more exact molecular-mechanical model (MM) is planned. Secondly, it remains an issue to design for effective two-handed interaction. More attention can be paid to the use of the dominant and non-dominant hand. Most often, the dominant hand will hold a tool, for instance the Gripper, whereas the non-dominant hand will hold a work-piece, for instance the cube.

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