Teaching Electronegativity and Dipole Moment in a TUI

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Abstract

This paper describes how a Tangible User Interface (TUI) that was designed to construct molecules was extended to also visualize electronegativity and dipole moment. Using interactive tools working with the system, elements can be chosen from a booklet menu and composed into three-dimensional (3D) molecular models. The system is used to teach aspects of organic chemistry such as the octet rule. Based on user experience and expert interviews, a new mode to visualize electronegativity and dipole moment was realized. Evaluation of usability and the learning effectiveness of the AC system is in progress, also examining the dipole tool presented here. We currently compare AC with a ball-stick tool for chemistry education. The paper is an example of joint disciplines: Tangible UI, educational media for chemistry education, and interactive learning.

1 Introduction

Electronegativity of an atom is the tendency of that atom to attract electrons. Electronegativity may explain many characteristics that a molecule with that atom may have. The dipole moment of a molecule is often drawn as an arrow, with the head pointing toward the more electronegative end. Negative and positive ends can be denoted as δ- and δ+. The polarity of a polyatomic molecule can be expressed in terms of its dipole moment which is a vector sum of all bond dipoles of the molecule. For complex molecules, a sum of the dipole vectors will give the overall dipole of the molecule.

Taking an augmented reality approach, an interactive application for the handling of three-dimensional (3D) molecular models was realized [1][4]. The application, which is a Tangible User Interface (TUI), is called Augmented Chemistry (AC) (Figs. 1-2). The AC system is already in use to teach certain aspects of organic molecular chemistry such as the octet rule. The following section describes the features and use of AC, interaction form, system set-up, and basic and specialized interactive tools. This is followed by the main section, showing how interviews with a chemistry teacher, also a user, led to a conceptual solution, followed by realization of 3D interaction with electronegativity and dipole moment.
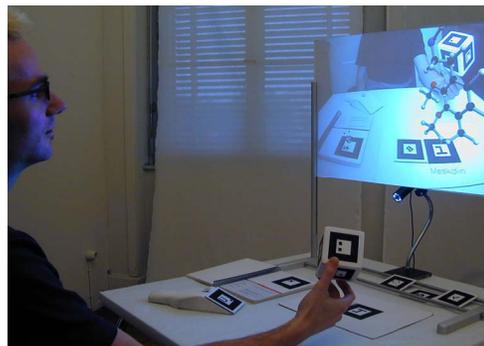

Figure 1. A user of AC viewing ball-stick representation of a composed molecule while rotating it with the cube.

Each kind of molecular model is meant to show a different aspect of chemistry and must be chosen depending on the educational purpose. For reasons of graphical coding and educational scope, a *ball-stick* model together with a standard color-coding is mostly used in the AC system.
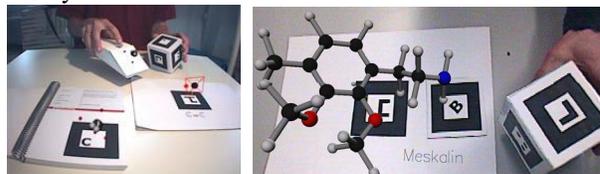

Figure 2. Left: Moving the gripper close to the booklet loads it. Leading the gripper to the platform and pushing its button, places the atom onto the platform. Right: AC employs standard color-coding for ball-stick representation of mescaline ($C_{11}H_{17}NO_3$): Carbon black, Oxygen red (here: gray), and Hydrogen white.

2 The TUI: Augmented Chemistry

AC is a workbench offering its users the opportunity to interact with virtual 3D molecular models in a direct way [1][4]. The system also offers tools to build composite molecular models. Following the conventional implementation of the AR Toolkit [2][3], interactive tools carry one or more fiducial markers, connecting a tool to an animated 3D model so that both tool and model can be seen in a composite image. Hence, chemical rules can be formulated and integrated into the application.

A booklet shows elements by a printed picture and a name. One hand browses the booklet, offering one element per page. Using a gripper, users can pick up elements from the booklet. Bringing the gripper close to the element in the booklet loads the gripper with that element. When the gripper has been loaded, it is positioned next to a platform. With the rotation of a cube, users can determine where and how an element shall connect to the molecule. Pushing a button at the gripper makes the loaded atom connect to the molecule at the platform (Fig. 2).
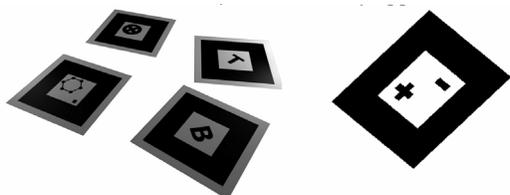

Figure 3. Markers, each representing a tools: Left: browser (front), tag-toggle (right), cleaner (behind), and benzene-template (left). Right: Dipole tool.

A set of specialized functions was realized as cards, becoming active when drawn onto the platform and each triggering one of the following tools: browser, tag-toggle, cleaner, and benzene-template [4]. A new specialized tool called *dipole* (Fig. 3, right) was recently implemented and is presented in this paper. The *dipole* card triggers a further viewing mode, visualizing electronegativity and dipole of the constructed molecule. While the dipole tool is effective during the entire construction sequence of a molecule, it makes most sense to chemistry education when a user has successfully constructed a predefined molecule.

3 Electronegativity and Dipole Moment

After a first interview with a subject-matter expert for chemistry education, who is also a user of the system, it was decided to extend the AC system to represent electronegativity and dipoles. After an Internet search and after having consulted a chemistry textbook, we found: To compute electronegativity, two fundamentally different alternatives were available. Either, a static implementation, requiring a molecular library to manually input charge distributions. Or, a dynamic implementation, calculating the polarity from the atom's features during molecule construction. The dynamic solution requires that some additional information about each atom is made available for real-time use. Given these alternatives and after a second interview, it came out that the dynamic model was most suited to the chemistry teacher's needs. Hence, the next step was to specify the 3D graphical

representation of electronegativity and the dipole moment based on a dynamic model.

To visualize electronegativity, two alternatives were available. Either, to use different color-coding (red for positive, blue for negative, and white for neutral) and color saturation. Or, a representation of molecular bindings with free flying electrons around each atom and with more electrons on the places with greater electronegativity. Since the latter alternative would require more programming and was less in line with standards for chemistry education, the former was chosen (i.e. color-coding and -saturation).
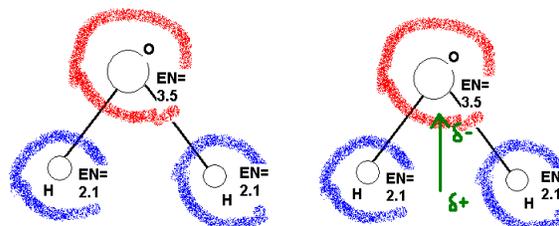
3.1 Conceptual Solution

Figure 4. Color-coding of electronegativity (EN). δ- and δ+ denote charged ends, connected by a vector (right).

In a first step, additional information necessary for each atom must be made real-time available. This information is electronegativity (see for instance Fig. 4), which can be found in tables in chemistry textbooks. Hence, it is possible to show a colored cloud around each element. The color of a cloud is determined according to relative electronegativity difference between elements in molecule (Fig. 4). If there are more than two electronegativity values, the color of clouds can be chosen from a scale of different saturations, such as deep red, light red, white, light blue, deep blue. In a second step, the dipole moment of the molecule is computed and visualized. Dipole moment is the vector sum of all bond dipoles of the molecule and can be calculated by employing vector algebra. Therefore, coordinates of each atom also have to be real-time available to the system. Dipole μ is the product of a partial charge (δ) and distance (d), see equation (1).

$$\mu = \delta * d \qquad (1)$$

3.2 Color-coding of Electronegativity

A function sets the colors of atom spheres as well as the dipole vector. First, the function loops over all elements globally available and records the maximum and minimum electronegativity values (global bounds).

Second, the function loops over all atoms in the currently constructed molecule and records the maximum and minimum electronegativity values (molecule bounds). With these bounds recorded, electronegativity color-coding is defined. Atoms with equal electronegativity are equally color-coded, even if they appear within different molecules. Coding of the color goes from blue, through white, to red. Coding of the saturation depends on molecule bounds in relation to the global bounds. Besides showing the location of positive and negative ends, such coding also shows the amplitude and inner relation among charges. Color-coding of the dipole vector also depends on the molecule bounds (Fig. 5).

3.3. Vector Direction, Length, Color-coding

For each pair of connected atoms, atom a and b, a local dipole vector is computed. The local vector's direction is a function of the two atoms' position and electronegativity, pointing from the atom with the greater to the atom with the smaller charge (Fig. 4). The length of the local dipole vector is given by equation (2).

$$\text{dipole vector}_{ionic} = \text{distance} * \text{charge difference} \quad (2)$$

As a first approximation, we estimate the distance to 1 and the charge difference to 1 for single bond, 2 for double bond, and 3 for triple bond. These are not values corresponding to the underlying physical model, but sufficient for a correct visual representation.

In a closer approximation, we compensate for the fact that equation 2 only is true for purely ionic connections. In the work presented here, covalent bonds are more in focus. Hence, we employ the method of Pauling in order to get a better estimate for the actual dipole vector, given by the compound equation (3).

$$\text{dipole vector}_{Pauling} = \text{dipole vector}_{ionic} * P \quad (3)$$

$$P = 1 - e^{0.25(electronegativity_a - electronegativity_b)^2}$$

For all pairs of connected atoms, local dipole vectors add up to the dipole vector of the molecule (superposition). The color of the molecule dipole vector is defined once only and follows the algorithm for color-coding of electronegativity. The *dipole* tool may be used separately or combined with the *tag-toggle* tool giving the name of each atom (e.g. H and O) (Fig. 5). Color-coding, color-saturation, and dipole vector can vary considerably (Fig. 6). An offset makes the dipole vector stand out from the atom spheres of the molecule. Offset was realized

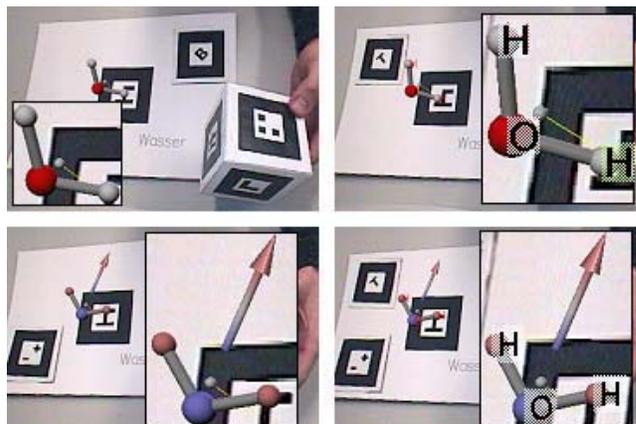through an algorithm looping over all the atoms of the molecule.

Figure 5 (top to bottom, left to right; focus framed with emphasized letters, for print reasons). Water (H$_2$O) in normal viewing mode (1st picture), using tag-toggle tool (2nd picture), using dipole tool (3rd picture), and combining tag-toggle and dipole tools (4th picture).
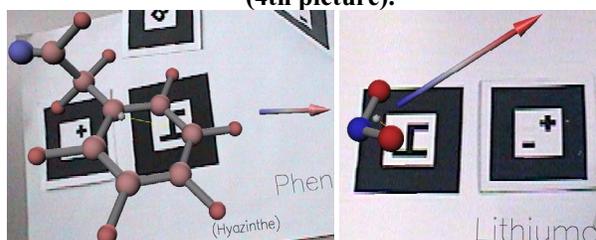

Figure 6. Color-coding, color-saturation, and dipole vector differ from phenyl acetaldehyde (C$_{11}$H$_{17}$NO$_3$) (left) to lithium oxide (Li$_2$O) (right).

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