Augmented Chemistry: Interactive Education System

Samarth Singhal
Computer Science Department,
Jaypee Institute of Information Technology, Noida, India

Sameer Bagga
Computer Science Department,
Jaypee Institute of Information Technology, Noida, India

Praroop Goyal
Computer Science Department,
Jaypee Institute of Information Technology, Noida, India

Dr. Vikas Saxena
Assistant Professor, Computer Science Department
Jaypee Institute of Information Technology, Noida, India

ABSTRACT
Current knowledge delivery methods in education should move away from memory based learning to more motivated and creative education. This paper will emphasize on the advantages tangible interaction can bring to education. Augmented Chemistry provides an efficient way for designing and interacting with the molecules to understand the spatial relations between molecules. For Students it is very informative to see actual molecules representation 3D environment, inspect molecules from multiple viewpoints and control the interaction of molecules.We present in this paper an Augmented Reality system for teaching spatial relationships and chemical-reaction problem-solving skills to school-level students based on the VSEPR theory. Our system is based on inexpensive webcams and open-source software. We hope this willgenerate more ideas for educators and researcher to explore Augmented Reality technology in the field of interactive education.

General Terms
Augmented Reality, Chemistry, Computer Vision, Computer Graphics

Keywords
3D Molecule, VSEPR theory, Fiduciary Marker keyboard, LED Glove, Augmented Reality Education

1. INTRODUCTION
The use of technology in education enables learning process to be more active, attractive, motivating, simulating, and meaningful to the student[1].For example, PowerPoint presentations, animated videosare being used pervasively in classrooms around the globe. The problem with this technologyis that the student remainsa passive element of the learning process. These Information Technologies must aim for better and more participationfrom the students. Augmented Reality (AR) as an advanced technology that enables user to interact with virtual and real world in real time application [2] can bring more natural experience, raises attention and motivation ofstudents with a high potential to enhance the learning experience [3, 4]. AR can also enhance the effectiveness and attractiveness of teaching and learning for students in real life [5, 6, 7]. AR systems may be used by multiple users at the same time. This provides the opportunity for collaborative applications, like engineering design, architecture, multi-user games, and education, among others.

We observed that many school going students have problem in learning and understanding molecular structures. This may be attributed to thelack of visualization of the spatial structures of the molecules which they are taught in a two dimensional representation on the blackboard or books. Understanding chemistry depends on understanding the spatial structures of the chemical parts.If the spatial structures and dynamic behaviour of the chemical molecules is conveyed to the students, chemical processes and chemistry per se canbe better understood.

We are interested in applying AR to Chemistry education at the school level. Specifically, lettingthemsee different elements and their reactions with other elements.Our Tool forms molecules based on Valence Shell Electron Pair Repulsion (VSEPR) theory. The goal is for them to gain a spatial intuition of the structures, a key skill for the students to understand and solve Chemistry problems.

Although the system has been developed for Chemistry, other disciplines may benefit from our system. For example, it can be applied to mathematics, organic chemistry, theoretical physics, astronomy, applied physics and engineering. Its simplicity and ease of use make it suitable not only for university students but also foryounger students, like highschool and secondary school students. It can also be used for demonstrations at fairs and trade shows, allowing prospective customers to interact with a certain product in a collaborative way.

2. THEORETICAL BACKGROUND
2.1 VSEPR Theory
Valence Shell Electron Pair Repulsion theory (VSEPR)theory is a model in chemistry used to predict the shape ofindividual molecules based upon the extent of electron-pair electrostatic repulsion. [8]

Generally, the "AXE method" of electron counting is applied before conducting the molecular structures based on the VSEPR theory. The VSEPR theory can be used to anticipate the shapes of simple molecules by applying a set of simple rules: (1) determine the number of valence electrons of the central atom (A), (2) identify the number of bonds between the central atom and outer atoms (X), (3) count thenumber of lone electron pairs surrounding the central atom (E), (4) determine overall geometry by the mutual repulsion between the electron pairs, and (5) final adjustments of the geometries such as slightly changing angles due to higher forces of lone electron pairs. Forexample, Methane (CH_4) contains one atom of Carbon (C) and four atoms of Hydrogen (H). It can be represented in "AXE" as AX_4 which means there is one central atomC, four valence electrons H and none of lone electron pair. An example of AX_4 geometry is "Tetrahedral" as shown in Figure 1.
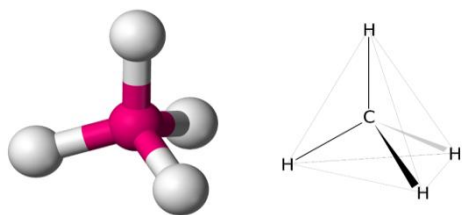
Fig 1: Tetrahedral molecular structure of the Methane

The atomic geometries can be found in many forms including Trigonal planer, Trigonal bipyramidal, Linear, Tetrahedral, Octahedral, etc.

2.2 Augmented Reality in Education

The basic principle of augmented reality is: through the sensor, the virtual scene and the real world organicintegrated, creating a realistic scene, which can greatlyenhance the immersiveness and interaction withvirtualenvironment [9].The basic procedure of augmented reality is:calculate the affine transformation of virtual model tocamera plane, according to the location of the camera andmarker information in the real world. Then, draw virtualmodel on the basis of affine transformation matrix. Finally, combine the video of real world and virtualmodel, displayed on the terminal display. Today AR is a matured technology whereearly surveys date back more than one decade [10]. Books have also been published entirely devoted to its study [11] [12]. Despite its maturity, it has barely been applied to education.Many processes, ideas and concepts can be better illustrated using both images of the real world and graphics. In this section we present the benefits of using AR in education includingthe survey of previous work in this area.

School teaching methodologies have not evolvedmuch for centuries. Recently, new technologies have appeared in the classroom. For example, it is common to see PowerPoint presentations and use networked platforms like Moodle [13]. Using these new technologies does not imply an increased interaction between students and the teachers. In fact, many times information keeps on flowing in just one direction, from the teachers to the students. For students to learn more and better, education has to be both experimental and interactive. We learn more from hands-on experiences than from traditional lectures. AR is mature enough to be applied to many every-day activities. Education is one of them, especially for the following reasons [14]:

    a.   AR supports seamless interaction between real and virtual environments.
    b.   AR allows using a tangible interface metaphor for object manipulation.
    c.   Finally, AR provides the ability to transition smoothly between reality and virtuality.

AR can also be used for online education. Project MARIE (*Multimedia Augmented Reality Interface for E-Learning*) uses AR to present 3D information to the students [15].

2.3 HSV Color Space

RGB (Red, Green, and Blue) is a widely used color space but HSV (Hue, Saturation, and Value) is sometimes preferred. Hue is a specification of theintrinsic color. Saturation, describes the purity of color. The last component ofthe HSV triple is a measure of brightness of color.

The advantages of HSV over RGB are:

    a.   Hue is invariant to certain types of highlights, shading, and shadows

    b.   The segmentation is performed on only one dimension (H) and results ofsegmentation have fewer segments than using RGB

3. DESIGN AND DEVELOPMENT

The basic purpose of project is to help increase the understanding of 3-D chemistry modelling and spatial arrangement of molecular structures in space. With the help of advanced AR technology (e.g. adding computer vision) the information about the surrounding real world becomes interactive and digitally tractable. In this project we want the students to intuitively build the molecular structures based on their chemical formulae, so we propose to use the AR technology for exhibiting the models. The layer of the model will be superimposed on a fiduciary marker. Apart from the rotation through the markers along z-axis, a cube consisting of six markers is provided to rotate the 3D model along x, y and z axes. For this we will be using ARToolKit library (HTLab, 2007) [16] which allows marker identification, position and orientation calculation.
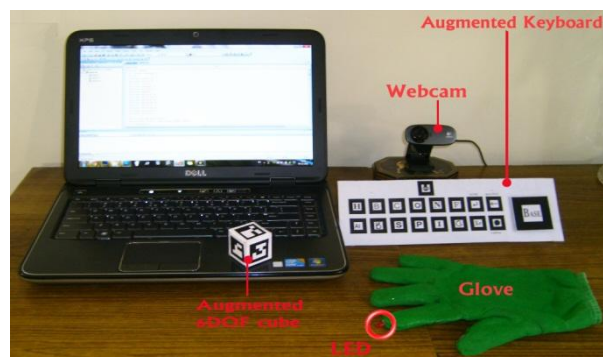

Fig 2: The Initial setup of the Project

For the purpose of input, a keyboard of markers is designed which will help the user to effectively select the atoms to form a desired molecule as shown in figure 3. The marker pattern in the keyboard have been designed to keep each key unique and distinguishable [17]. The user has to click on the requisite marker for the element to be added to the base marker. To register a click on the selected element we have defined a simple gesture using the thumb and fore-finger as shown in figure 4. This gesture completes the LED circuit and it glows at the tip of the fore-finger. The element which the forefinger is pointing to is selected. The LED tip is detected by analysing image for proper HSV color and getting the contour using OpenCV library, this is based on the Collision Detection and Direction finding [18]. To trigger the analysis of AXE model for the input set of elements we use enter key. Users are also provided with the marker to delete the most recent element added and clear all the elements and start afresh.This input method of keyboard and tangible interaction can be useful for other subjects.
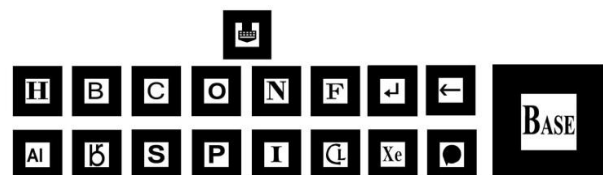

Fig 3: Fiduciary Marker Keyboard consisting of elements from the periodic table, Enter, Back and Reset keys along with Base marker.

Fig 4: LED Glove Hand Gesture

Our approach has the potential to help students design, learn and interact with chemical structural models and reactions in a better and intuitive way.

Experimental education is an important part of science teaching, in order to develop and train the scientific literacy of students. Experiments promote and enhance the process of scientific inquiry skills, so as to strengthen the students' ability of understanding and solving problem.

4. IMPLEMENTATION PROCESS

4.1 Click Detection

4.1.1 Detecting the user click position:
a. Search the current frame for LED bulb's HSV range
b. Find the contour of the selected colour
c. Estimate the centre of the contour (Xcentre, Ycentre)

4.1.2 Map these Centre coordinates with the Keyboard markers coordinates:
a. For each AR marker on the keyboard, its real 3D position with respect to camera is calculated using the Modelview matrix given by ARToolKit
b. C(x,y,z) = -R' * t , where ' is transpose   R is Rotation matrix (Modelview's upper left 3x3 matrix, transposed), t is Translation 3x1 matrix (in terms of right-up-back vectors)
c. We use C(x,y,z), Modelview matrix, Viewport matrix (Viewport matrix is 1 by 4 matrix, used in OpenGL: [x, y, width, height] x,y specify coordinates of lower-left point on user's screen, usually x=0, y=0, width and height specify inner width and height of OpenGL window) and Projection matrix with perspective initialized to 45° to obtain the screen coordinate of key marker (posX,posY) using OpenGL function gluProject().
d. Find the minimum sum of
$$\left(abs\left(Xcentre - posX \right) + abs\left(Ycentre - posY \right) \right)$$
among all the key markers and save its index as hit.
e. Also obtain the range among all the coordinates of key markers to get the maximum area under which a click can be registered i.e. range of x, y coordinates from centre of marker under which we will be looking for a key press match:
   i. First we get the position of (min, max) value of (x,y) coordinates among all the keys these are labelled as (minkx, minky) and (maxkx, maxky)
   ii. Along with x coordinate of (min, max) we also get the index of (min, max) keys of keyboard and store them as (rxmin, rxmax)
   iii. Also as keyboard has 2 rowsof 8 keys thus rxmin needs to be adjusted depending on how keyboard is placed in front of camera as (maxkx- minkx) is normalized by dividing by (rxmax-rxmin) to reflect width of 1 key, thus:

$$rangex= \frac{maxkx\text{-}minkx}{abs(rxmax\text{-}rxmin)}$$

   iv. To get height of a key:
$$rangey=(maxky\text{-}minky)$$
f. If the distance of hit marker from the (Xcentre, Ycentre) lies under the rangex &rangey then key hit is registered and the necessary operation is carried out

4.2 VSEPR Theory
The only inputs we have are atomic number, electronegativity and atomic radius of the atom selected from keyboard.Using onlythese inputs we need to determine the final molecular geometry.

4.2.1 Calculate Electronic Configuration:
a. The s orbital set contains a single orbital, and by Pauli's Exclusion Principle, *a single orbital can hold a maximum of two electrons,* so each s orbital set can hold two electrons
b. Similarly pcan hold 6 electrons, d can hold 10 electrons and f can hold 14 electrons
c. Orbitals are filled in the order of increasing n+l if same then they are filled in order of increasing n

4.2.2 Calculate Valency:
a. It is a measure of the number of bonds formed by an atom of a given element
b. For most elements the number of bonds can vary. As a general rule it is number of atoms it needs to lose or gain in order to attain the noble gas configuration
c. Valency changes during molecule formation due to electronegativity

4.2.3 Analysis of AXE:
The analysis of AXE contains three sub-procedures:

4.2.3.1 Find the central atom (A):
a. If both positively charged and negatively charged elements are present
   i. A is the element with highest magnitude of valency
b. Else If only negatively charged elements present
   i. A is the element with the least Electronegativity and maximumpolarity
   ii. A+=8

4.2.3.2 Find the number of surrounding atom (X):
The value of X in AXE is the number of atomsthat surrounds the central atom. All of theelements in the list are counted as 1 except thecentral element, in cases such as O_2, I_3^-; X is determined by counting number of atoms and subtracting 1 i.e.X= (no of atoms -1)

4.2.3.3 Find the lone pair electrons (E):
a. If both positively charged and negatively charged elements present
b. E=8-valency of A-valency of all the X
c. If E < 0
d. Find the maximum electronegativity atom
e. Decrease charge of maximum electronegativity atom by 1 and increase E by 1 till E is 0
f. If (E%2) != 0
g. Find the maximum electronegativity atom, *me*
h. If polarity of *me*> 0

i.   Reduce E by 1 and divide by 2
j.   Increase the charge of *me* by 1
k.   If polarity of me < 0
l.   Increase E by 1 and divide by 2
m.   Reduce the charge of *me* by 1
n.   Else
o.   E is divided by 2 and stored for model determination
p.   If only negatively charged elements present
q.   E = polarity of A – valency of all X
r.   If E < 0
s.   Find the maximum electronegativity atom
t.   Decrease charge of maximum electronegativity atom by 1 and increase E by 1 till E is 0
u.   If (E%2) != 0
v.   Find the minimum electronegativity atom, *me*
w.   If *me* is not the central atom
x.   Reduce E by 1 and divide by 2
y.   Increase the charge of *me* by 1
z.   Else
aa.   E is divided by 2 and stored for model determination

4.2.3.4 Determine Molecular Geometry

From the values of A, X and E VSEPR the model is determined

4.2.3.5 Formal Charges

Formal Charge = (Valence electrons)-(Assigned electrons)

4.2.3.6 Bonds

No of bonds=Valence electrons–mod(Charge)

4.3 Other Components

4.3.1 Occlusion Removal:

a.   Search the current frame for glove's HSV
b.   Save a mask of this particular colour
c.   Pass this mask into OpenGL and display it over a transparent Quadrilateral, blending it such that only Glove pixels are visible

4.3.2 Rotation Cube:

a.   It consists of 6 markers, numbered 1-6
b.   The Model rotates according to the markers visible to the camera. If two markers are visible at a time then it rotates only in 2 axes. And if three markers are visible at a time, it rotates in the entire three axes as per the cube's position.

Fig 5: The augmented markers rotation cube

5. RESULTS

In our interaction with various school students we concluded the major problems in understanding 3-D structures in VSEPR theory were related to difficulty in visualising the spatial arrangement of different atoms in 3-D space, bond formation and type of bonding among different atoms of molecule and bond angle and lone pair influence on the existing bond. In Augmented Chemistry our purpose was to solve these problems in a manner in which we can develop among students a much greater understanding and interest for the topic. The fiduciary marker keyboard coupled with hand glove with LEDmakes the input easy and interactive. The setup of the program is inexpensive with only webcam, glove and LEDas external requirements. It is portable and can be setup anywhere without much ado.
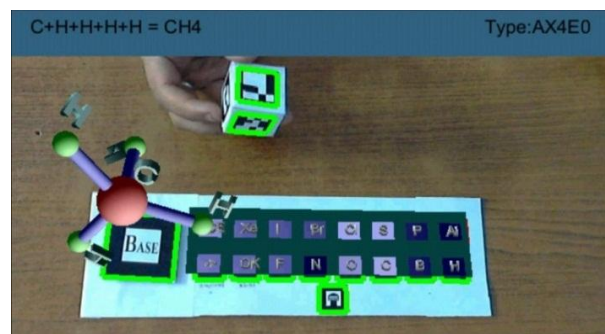

Fig 6: Methane (CH$_4$) molecule being rotated by the cube

6. LIMITATION AND FUTURE RESEARCH

Visitors who have used it at exhibitions where program was exhibited have reported some of the limitations and problems. Future research will be conducted to solve these problems. The following are some of the limitations:

a.   Dependence on Light: Use of fiduciary markers and vision makes it mandatory for us to have decent amount of lighting too dark or bright a surrounding can hamper the input and output module.
b.   Molecule formation process: Currently the program is unable to communicate the whole process with step by step explanation to the user, also the details ofthe changes in bond angle due to Lone pair and Bond pair repulsions have to be included.
c.   Complex molecular structure: Many visitors demand the program to be able to display complex molecular structures such as the Benzene (C$_6$H$_6$), Caffeine (C$_8$H$_{10}$N$_4$O$_2$). These compoundsbelongs to organic chemistry, which is out of our scope. In order to perfectly form these molecular structures, other chemistry theories are required.

7. CONCLUSION

We have introduced an AR system for teaching Chemistry at high school level. Our system uses inexpensive cameras and open-source software to set up a collaborative environment that supports several groups of students interacting with elements and compound structures. Interaction is handled using hand-held markers and ARToolKit a public domain AR software library, which will allow us to deliver this program to other institutes/schools for educational purposes. Our experience with the system during variousexhibitions shows that the students enjoy it and gain more knowledge of molecular structures. We have also observed that they substantially improve their spatial intuition and learn to better understand visual cues.

The VSEPR theory in itself is sufficient for the covalent bonding molecular structures, the program must be expanded to cover other types of bonding structures in Chemistry, as well as disciplines like Mathematics, Physicsand Engineering applications. We also want to improve the tracking and rendering capabilities of the system. The overall objective is to be able support more students and have a classroom permanently outfitted for collaborative AR education.

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