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Development of "Functional Groups in Molecules" Models For Fundamental Science Curriculum

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ABSTRACT

In order to teach quantum concepts to primary school students, new molecular models have been developed to better visualize a few typical molecules. Both computer and physical molecular models particularly those displaying functional groups were created from Atoms in Molecules (AIM) theory. The surface of each model was calculated from 0.01 atomic unit (au) electron density surface of the molecule. MORPHY was used to calculate an inter-atomic surface (IAS), and several software programs such as Gaussian, VMD, Points2Polys, and Vizx3D were utilized to create three dimensional models. Different functional groups were colored, and connections between the functional groups were shown by IAS. The final physical molecular models were prepared by a rapid prototype machine at Thailand National Metal and Materials Technology Center (MTEC).

Keywords: Molecular models, X3D, Atoms in Molecules theory, functional groups

INTRODUCTION

Today's global economy has driven educational reforms worldwide in order to improve the economic productivity of the labor force, especially work specialized in science and technology. Science-oriented education and problem-solving skills seem to have the highest impact on economic growth. However, the education system in Thailand lags behind many countries in the region, especially in science and technology, an area crucial for national competitiveness and creative problem-solving [1]. Thus reform of science education provides an instant solution to enable the country to compete in this knowledge-based global economy.

Since 2000, a fundamental science curriculum [2] has been developed by the Institute for the Promotion of Teaching Science and Technology (IPST) in Thailand. This prototype curriculum is different from other Thai primary school curriculums in both content and teaching procedure. The curriculum does not emphasize the content but rather a few simple principles. One of the principles is the quantum state. The quantum state can be easily seen in macroscopic system such as the state of a cat (dead or alive) [3]. However for something small and naturally invisible, such as atoms and molecules, computer models are necessary. Well known models are "ball-and-stick" and "space-filling" representations. The classic ball-and-stick model represents atoms as colour-coded spheres and bonds as cylinders to emphasize molecular connectivity, while "space-filling" representations, such as a CPK (Corey-Pauling-Koltun) surface [4], highlight the overall shape and contours of a molecule. These models are usually used by scientists and students in universities and high schools. However, both types of model suffer from overcrowding, in that the overall molecular structure is swamped by the atomic detail. Moreover, they represent limited information such as the position of atoms and bonds in a molecule. For molecular shape, the iso-surface model is better at displaying the real shape, but the position of the atoms cannot be visible except if the surface is semi-transparent. The semi-transparent surface can be easily achieved by a computer model. For a physical model, it is more difficult. Furthermore, there is a theory that can define the atom better. AIM theory [5], invented by Richard F.W. Bader, connects quantum mechanics and standard chemical concepts such as atoms and a chemical bond.

In Schrödinger's equation, there is no explicit concept of an atom or a bond. It is only concerned with electrons and nuclei in potential fields. In contrast, standard chemical knowledge is based on the atomic model. So on one hand the rigorous and physically correct quantum mechanics calculations is required and on the other hand simple models related to conventional chemical intuition is needed. AIM theory is unique in the sense that it provides a rigorous link between intuitive chemical concepts and quantum mechanics through analysis of the electron density. Two other theories, used to calculate atomic properties, are partitioning of orbital space, and partitioning of the Hamiltonian but they do not provide a concomitant picture of the atom's shape. Rafat and co-workers [6] employed

this theory in rendering of quantum topological atoms and bonds for more complex molecules. Utilizing AIM theory one can define an atom in a molecule and the concept of functional groups can also be achieved.

The study of the characteristic chemical properties of many molecules with very diverse chemical structures has led to the introduction of the functional group concept - a group of atoms causing the molecule to have certain "functions" (i.e. the capacity of participating in specific chemical reactions). During a specific reaction the structure of the functional group changes while the rest of the molecule remains unchanged. From a structural point of view the functional group is a group of atoms connected by certain types of chemical bonds. In the last 150 years a large list of functional groups has been created, i.e. the relationship between the structure of molecules and their properties was discovered. In our study, some simple molecules were modeled in order to teach quantum concepts to primary school students.

MATERIALS AND METHODS

In this section, we describe in detail our methods in creating models as shown in **Figure 1**. This section is divided into four parts: creating electron density and wave function data, molecular surface construction, inter-atomic surface (IAS) construction, and creating the final model.

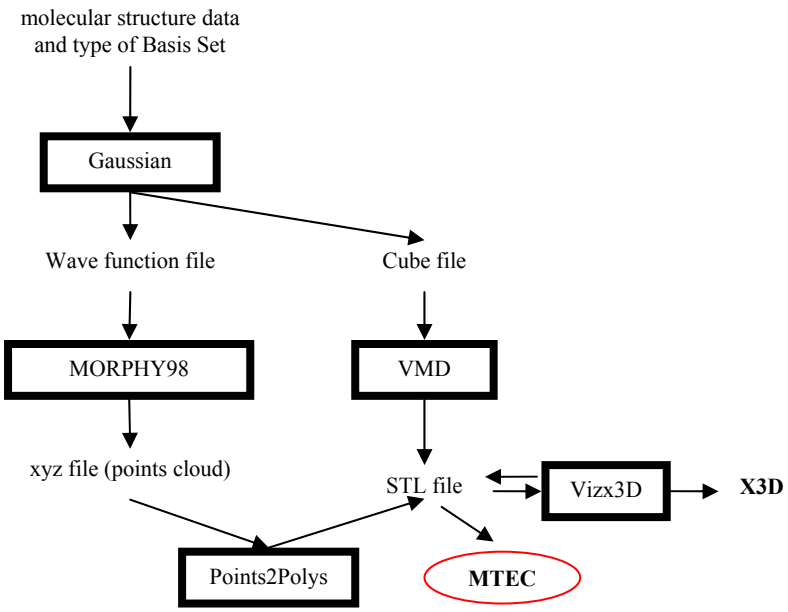


Figure 1 A diagram presenting steps in creating the models.

1. Creating electron density and wave function data

The static molecular structures of molecules were collected either from experimental or theoretical data sources [7-9]. Generally, they were types of atoms and their positions in space. This information together with the calculation method and type of basis set was employed as the input for Gaussian [10] to generate wave functions and cube files. Electron density was stored in the cube file format. An example is shown in **Figure 2**.

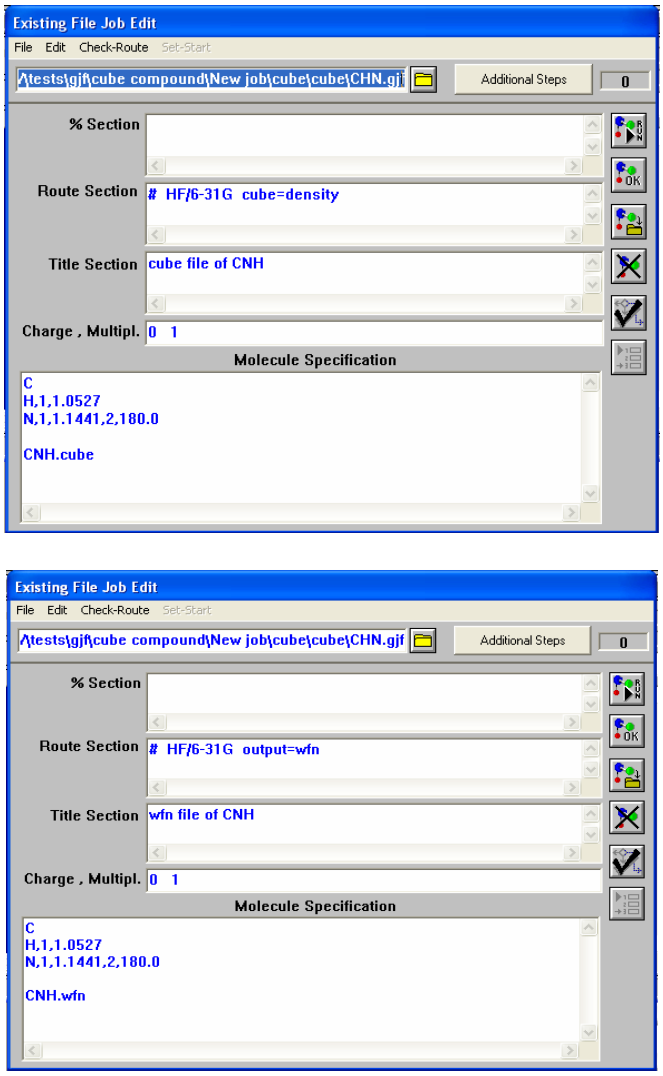


Figure 2 Gaussian inputs for creating (top) cube file (bottom) wave function files.

2. Molecular surface construction

This surface is the iso-surface of molecular electron density. Many programs are able to create this surface. However, VMD [11] was selected because it can export the surface as a stereolithography (stl) file. VMD reads electron density data from the cube file and creates an iso-surface at 0.01 au. This value was the optimum value. At 0.001 au the molecule was too big and the shape was not clearly shown.

3. IAS construction

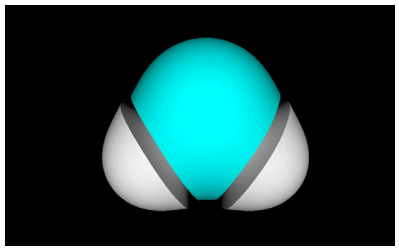
Morphy98 [12] was able to calculate the coordinates of points or point cloud that represent the IAS from the wave function file. The result was a text file with extension xyz. The point cloud was then converted into a polygon surface by Points2Polys [13] and saved as a stl file.

4. Creating the final model

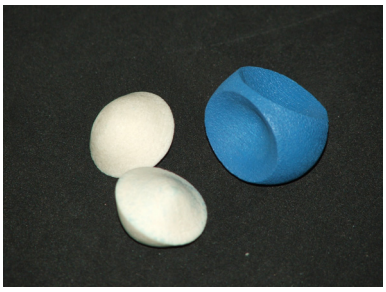
The final model was created by Vizx3D [14]. It imported the surface of the whole molecule from step 2 and divided it into smaller parts with the IAS from step 3. The result was smaller parts well-known as functional groups. These functional groups were then converted into X3D [15] extensions that can be accessed from a Web Browser. They were also converted into stl files that were prototyped using the rapid prototype machine at the Thailand National Metal and Materials Technology Center (MTEC) [16].

RESULTS AND DISCUSSION

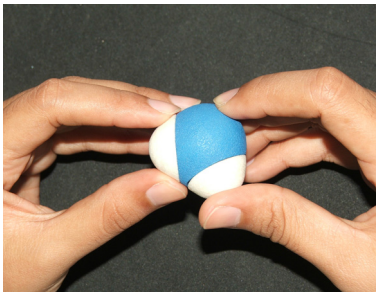
A simple molecule such as water was used to demonstrate AIM theory. The X3D model is shown in **Figure 3 (a)**. In the figure, water consists of a blue oxygen atom with two holes and two white hydrogen atoms with a bump. There was a gap to separate the hydrogen and oxygen atoms. The real model was shown in **Figures 3 (b)** and **(c)**. The holes and bumps are clearly shown in **Figure 3 (b)**.



(a)



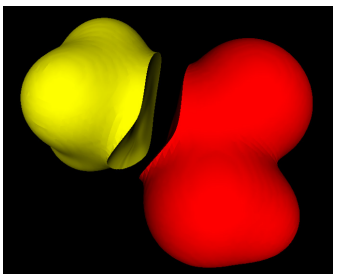
(b)



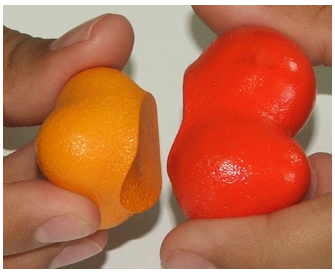
(c)

Figure 3 Water molecule (a) X3D (b) separated model (c) joined model.

One of the most common organic acids is vinegar or acetic acid. The X3D and real models of acetic acid are shown in **Figures 4 (a)** and **(b)**, respectively. The carboxylic group is shown in orange and the methyl group in yellow. The real methyl group did not have exactly the same color as the X3D model because of the limitations in real color.



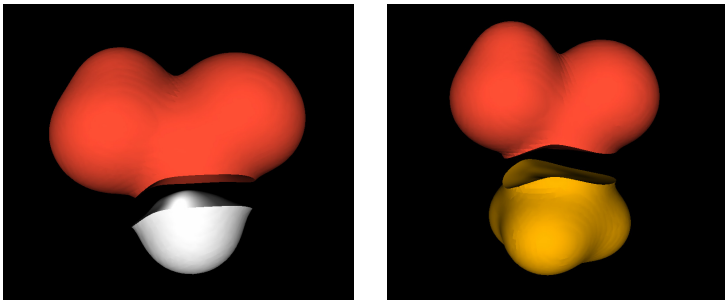
(a)



(b)

Figure 4 Acetic acid (a) X3D and (b) real model.

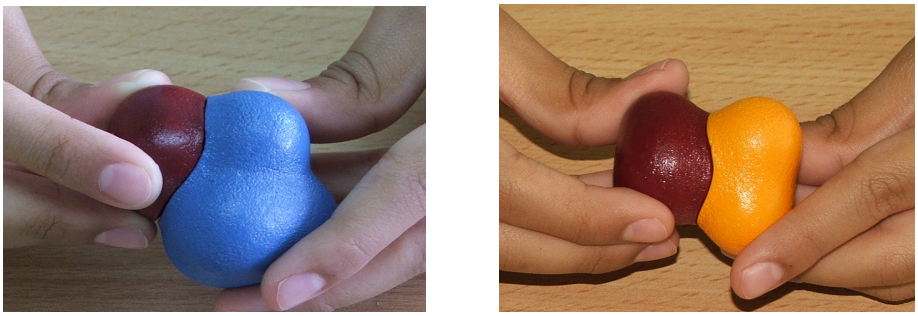
For molecules with the same functional group but different side chains, the X3D models are shown in **Figure 5**. These are formic acid and acetic acid respectively. The differences between these two acids are in the side chain and IAS. The side chain of formic acid is a white hydrogen atom. For acetic acid, the side chain is a yellow methyl group.



(a) (b)

Figure 5 X3D model of formic acid (a) and acetic acid (b).

One of the best known functional groups is the hydroxy group, shown in **Figure 6**. Two molecules, methanol and ethanol, were chosen to model this functional group. The different side chains were the blue ethyl group and the yellow methyl group. The hydroxy group is represented in dark red.



(a) (b)

Figure 6 (a) Ethanol and (b) methanol.

From above examples, the model was able to demonstrate the correct shape of the molecule such as water's round shape instead of v-shape as shown with a ball and stick model. For more complex molecules, the real shape was also easily visualized. However, the high cost of prototyping is a limitation. The unique shape of functional groups in a molecule also limits the reusability with similar molecules when compared with a ball and stick model. Although they were the same functional groups, their shapes were not exactly the same. This was clearly shown by the different IAS in **Figure 5**. However, the topology of the IAS will arouse the interest of students and give more insights into the chemistry of chemical bonding. Bonding is generally classified as either ionic or covalent. But most bonds have both ionic and covalent characteristics. These characters could easily be visualized from the topology of the IAS. The curved and flat surfaces represented ionic and covalent bonding respectively. Each IAS might have both of these characters.

CONCLUSIONS

From AIM theory, both computer and real models were created for quantum state teaching. This unique model will help students in understanding the concept of atoms, molecules, and bonding. In the future, with mass production of plastic models, the cost will be lower and with magnetic implantation at IAS, temporary binding of functional groups to form a molecule can be achieved.

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บทคัดย่อ

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การพัฒนาแบบจำลองหมู่ฟังก์ชั่นในโมเลกุลสำหรับหลักสูตรวิทยาศาสตร์รากฐาน

แบบจำลองแบบใหม่ของโมเลกุลง่ายๆ สองสามชนิดได้ถูกสร้างขึ้นมาเพื่อใช้ในการสอนแนวคิดทางควันตัมกับนักเรียนประถม แบบจำลองบนคอมพิวเตอร์และแบบจำลองจริงที่เน้นการแสดงหมู่ฟังก์ชั่นได้ถูกสร้างขึ้นจากทฤษฎีอะตอมในโมเลกุล โดยพื้นผิวของแบบจำลองได้มาจากค่าพื้นผิวของความหนาแน่นอิเล็คตรอนที่ 0.01 atomic unit (au) ของโมเลกุล ส่วนพื้นผิวระหว่างอะตอม (IAS) ถูกคำนวณด้วยโปรแกรม MORPHY นอกจากนี้ยังมีโปรแกรม Guassian, VMD, Points2Polys, และ Vizx3D ที่ถูกใช้ในกระบวนการสร้างแบบจำลองหมู่ฟังก์ชั่นต่างชนิดกันจะถูกให้สีต่างกันและการเชื่อมต่อกันระหว่างหมู่ฟังก์ชั่นถูกแสดงด้วย IAS ในขั้นตอนสุดท้ายแบบจำลองจริงถูกขึ้นรูปที่ศูนย์โลหะและวัสดุแห่งชาติ (MTEC)

สำนักวิชาวิทยาศาสตร์ มหาวิทยาลัยวลัยลักษณ์ อำเภอท่าศาลา จังหวัดนครศรีธรรมราช 80161