

Description for structure of substances by computer 3D animation in chemical education

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Abstract: By means of computer 3D animation and multimedia technology, the basic concepts of chemical bonding theory (Valence Bond Theory and Hybrid Orbital Theory, including Van der Waals forces) and the structures of some typical inorganic and organic substances were vividly described to students using teaching software. The relationship between hybrid orbitals and the space structure of molecules was the focus in this software. The main contents, design ideology, and practice effects are introduced in this paper.

Keywords: structure chemistry, hybrid orbital theory, multimedia technology, space structure of molecules

Understanding chemical bond theory and the structure of substances requires significant knowledge of a number of topics, including atomic structure, molecular structure and crystal structure. These concepts are abstract and contain many details. Consequently, it is a teaching challenge at both the high school and college level.

A vivid three-dimensional animation and interactive stereoscopic model combines the contents of teaching material^[1-4], the atomic orbital, chemical bond, common molecules, ionic groups and typical crystal structures. Furthermore, it emphasizes the relationship between hybrid orbital theory and space configuration of molecules, an abstract concept that is often difficult to understand. This three-dimensional animation greatly increases the learner's studying interests and achieves excellent teaching effect.

1. Principle Contents and Design Ideology

1.1 Main contents of the software

The software consists of four components: atomic structure, chemical bond theory, molecular and crystal structure. (Fig 1). This structure is a hierarchy itself and matches the contents of the teaching material.

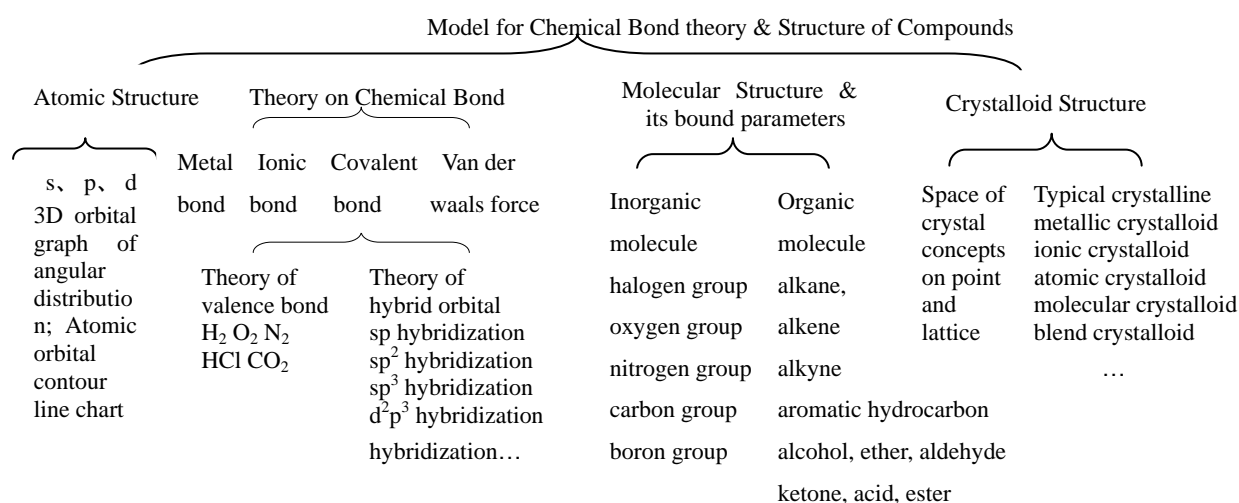


Fig 1 main contents and framework of the software

The shape of atomic orbitals, space-stretched and symmetric orientations are briefly shown in the atomic structure section. A three-dimensional atomic orbital angular distribution figure, which can be

interactively observed, is designed because the formation of the chemical bond and space configuration of the molecule are greatly effected by the angular distribution graph. There are s, p and d orbital angular distributions (**figure 2**) and contour lines that embody atomic orbital wave function:

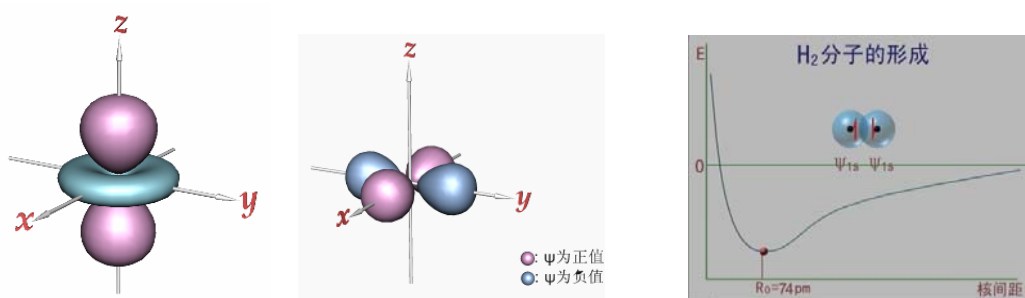


Fig 2 Contour representations of the two 3d orbitals Fig 3 The changes in potential energy during the formation of the H₂ molecule

Chemical bonds are classified into covalent, ionic and metallic bonds, etc. In order to make the software framework content succinct and integral, the intermolecular forces were linked to the model for chemical bond theory. In the software, three-dimensional animations for the molecular bonding process of hydrogen (H₂), hydrogen chloride (HCl), oxygen (O₂) and nitrogen (N₂) were designed to illustrate the main points of valence bond theory. The animation simulation demonstrates the system energy changes along with the distance between two nuclei in the process of hydrogen molecular bonding in (**figure 3**). Three-dimensional animations of hybridization and bonding of sp, sp², sp³, and d²sp³ (or sp³d²) hybrid orbitals are designed for hybrid orbital theory, respectively. The relationship between hybrid orbitals and molecular configuration is introduced by animation (**figure 4**). The formation of sodium chloride was used to illustrate ionic bonding. The model of dispersion force, induced force and orientation force is established to display intermolecular Van der Waals forces.

Molecular structure includes two sections, namely, inorganic molecular structure and organic molecular structure. According to elemental periodic table, halogen group, oxygen group, nitrogen group, carbon group, boron group, and other groups classified with their major inorganic molecules or ionic groups are introduced in the former section; based on the classification of functional group, main compounds are listed in the later section. These three-dimensional stereoscopic ball-and-stick models and corresponding structural formulas are designed and made for each molecule and include several parameters, such as bond strength, bond angle and bond energy.

The concepts of the close-packed ball model, point group Lattice, seven main crystal systems and some typical crystals are briefly introduced in crystal structure. For further details, it can be combined with multi-media teaching software—《crystal structure foundation》^[5] made by our research group.

1.2 Design ideology of the software

The advantage of computer multi-media technology is that it breaks through the traditional medium; it can integrate writing with many kinds of media such as text, image, sound and animation. The key factor in software design is selecting the appropriate medium for achieving the optimum teaching effect. The molecular structure and atomic crystal structure were expressed by the ball-and-stick model, while three-dimensional animation was used to exhibit specific space arrangements of atoms and the bond length and angle formed by the combination of atoms.

Adopting a full three-dimensional interactive form, the zoom, rotation and horizontal movement of

the model were executed by dragging the model with the mouse. The optimum design scheme is that the observers can view the model autonomously in all directions. As for the contour line graph of atom orbits and molecular structural formulas, two-dimensional images can be used to express them clearly. When a dynamic process, such as interatomic bonding and the interaction between molecules, is to be expressed, it can be described dynamically in the form of three-dimensional animation so that the observer can display the animation autonomously according to self-need. In addition to the picture, a detailed caption, music and oral explanation were attached to each part of the contents.

2. Technology Scheme of the software

2.1 Development tool

The creation of the model and animation were generated by 3D Studio Max in the software; all picture materials were edited and processed by Photoshop; atomic orbital contour lines and structural formulas of organic and inorganic molecule were drawn by Corel Draw; production of full three-dimensional interactive scenes was achieved by Quick Draw in the multi-media project.

The major framework of the software is assembled by Director 7.0; the software's starting interface is made by Visual basic; oval window is cut out by calling API function and then the animation of the begin segment is played in full screen; after the animation ended, the EXE file executed by calling Director program. The edition and composition of video animation, caption adding, format conversion and editing of background music are finished by Premiere. Dynamic special effect process of the buttons of the first segment, the last segment and interface are finished by After Effects.

2.2 Functional design of the software

The software can be run shortly after Quicktime is installed by the prompt. The first branch framework can be shown in the main interface; the second directory interface can be entered by clicking the corresponding button. There is a summary expounding the theory plate in this directory interface, branch title button can be selected to enter exhibition interface at the bottom (as shown in figure 4). There are three sub-windows in total: menu window, exhibition window for model animation and text window. Each of the windows can be arbitrarily moved or closed in order to organize the space of a whole page conveniently.



Fig 4 The software's simulation interface

The upper desktop can be returned by every lever-returning button. Moreover, there is display icon for control over background music in the main window. When clicking the button to exit, the software can be quit. The running of the software can be ended by clicking the "ESC" key at any status.

3. Features of the Software and Its Applying effect

The features and effects of the software can be illustrated by the formation of beryllium dichloride (BeCl_2) (as seen in figure 5). When beryllium dichloride (BeCl_2) is formed, the central beryllium atom forms two equivalent sp hybrid orbitals, which combine with the p orbitals of two chlorine atoms to form two equivalent Be-Cl bonds.

The electron filling state in the atomic orbitals is illustrated by transparency: opacity shows full filling of electron; semi-transparency reveals half filling, lucency indicates an empty orbital. As the orbitals hybridize, the s orbital is changed from opacity to semi-transparency, and the p orbital is transformed from lucency to semi-transparency (as show in figure 4b, c). Two transparent empty orbitals are hidden in the animation, emphasizing the hybridization of the s and p orbitals. In the software, the bonding in the BeCl_2 molecule is shown vividly by the change in orbital color, shape and movement of electrons, which are disappearing and appearing slowly. Abstract concepts and process are visualized and embodied by a virtual fluent animation model. It has an important impact on student understanding of the movement of atomic particles. Three-dimensional models for several typical molecules are shown in figure 6.

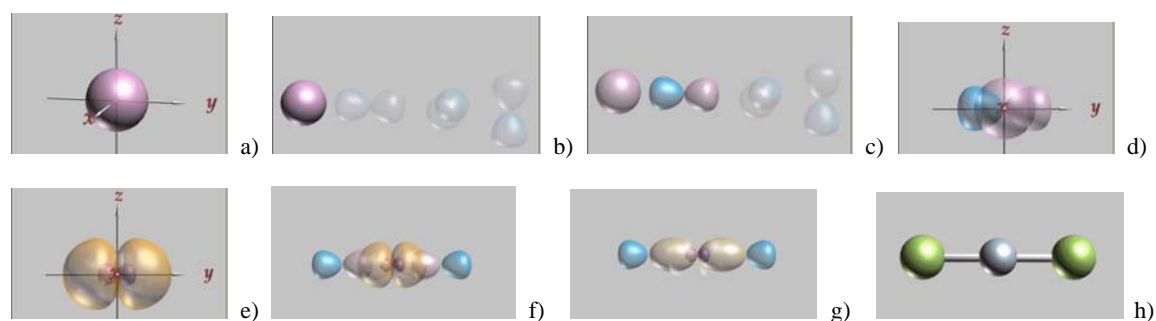


Fig 4 Formation of two equivalent Be—Cl bonds in BeCl_2

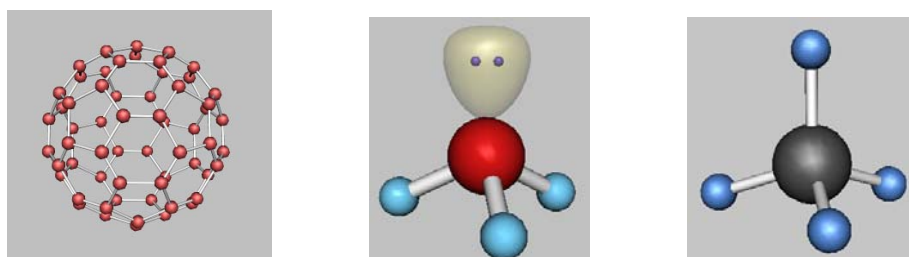


Fig 5 3D models of typical molecules a) C_{60} b) NH_3 c) CH_4

The fundamental theories and concepts of modern chemistry were described by vivid and visual three-dimensional dynamic stereoscopic model images and some simulative animation. So it will be of great help for students to deeply get to know and apprehend basic properties and structures of atoms and molecules. The software is convenient and powerfully interactive to use. In addition, its knowledge structure matches chemistry teaching material. So it is an important complement to the theoretical teaching of structural chemistry. In the chapter of “atomic structure and molecular structure” in fundamental chemistry and the course of structural chemistry, it has been used many times, and has got twice the result with half the effort.

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