# Student Visualization and Conceptual Understanding of Atomic Orbitals Using a Virtual Environment

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## Abstract

*In order to understand various aspects of student understanding of atomic orbitals, we have built a 3-D virtual environment – "Virtual Water" – to support the learning of some concepts of Physics and Chemistry at the final high school and first-year university levels. It is centered in the microscopic structure of water and explores, among others, concepts related to atomic and molecular orbitals.*

*We have made a qualitative study with twenty first year students of Science and Engineering courses at the University of Coimbra, Portugal. Being asked to describe their views about how they conceive electrons in an atom before seeing "Virtual Water", students revealed some misconceptions. We have tried, with partial success, to overcome them by making students explore the virtual environment.*

## 1. Introduction

There have been a number of investigations of students' misconceptions and their difficulties in understanding quantum mechanics. Much of the early work came from the Frankfurt, Bremen, and Berlin Groups in Germany. Further research has been carried out by Mashhadi [1], Styer [2], Johnston, Crawford, and Fletcher [3], Bao, Redish, and Steinberg [4], and Ireson [5].

On the other hand, various authors [6, 7, 8, 9] have defended the regular use of computer simulation and visualization in Physics and Chemistry teaching. They further argue that students should be given an active role in using these tools [10].

While there are an increasingly larger number of educational studies which focus on student conceptions of a specific set of topics at a given curricular level, there are far fewer attempts at probing how students' understanding of common or core topics are changing with the use of new visual pedagogical means.

At the beginning of the seventies Bordass and Linnett [11], Olcott [12], and Streitweiser and Ownens [13] were among the first to use computer-generated three-dimensional contour diagrams to represent atomic and molecular orbitals. However, these traditional presentations of orbitals as point distribution functions and contour surfaces are abstract and sometimes inaccurately simplified. The viewer has difficulties to visualize the true nature of the electron cloud, especially how diffuse or dense it actually is in different regions of the atom or molecule.

Since students are now much more routinely exposed at an early stage to new pedagogical materials, more sophisticated graphical representations are necessary. As a result, the presentation of the quantum mechanics core material has changed over the last years. Many of the most recent examples of modern course materials, including not only textbooks but also software, allow students to visualize quantum abstractions.

Some of this kind of software is the "Atomic Orbitals CD", by Y. Wong and Knowledge by Design [14], and the "Visual Quantum Mechanics", by N. Rebello and D. Zollman [15]. Both of them allow for visualizing atomic orbitals and electron densities. More recently, Cataloglu and Robinett have been exploring the development of student understanding in quantum theory to develop modern web-based instructional materials related to undergraduate quantum mechanics [16].

However, mostly of this software stood mainly on the creation of 2-D representations. Recent advances have created possibilities for 3-D visualization, which becomes increasingly important in learning scientific subjects like atomic orbitals. Therefore, the analysis of visualizations skills will likely be of increasing importance for testing the effectiveness of such new materials.

## 2. Virtual reality

Recent advances in visualization and computer technologies have created new possibilities in Physics Education for visualizing 3-D objects. One of the most promising means to support advanced learning environments for science education is virtual reality. This is a computer interface characterized by a high degree of immersion and interaction, which may make the user believe that he is actually *inside* the artificial environment.

The concept of virtual reality is not recent. It has been used for more than thirty years. However, only recent progress in hardware and software brought this technology to within the reach of ordinary users.

One benefit of virtual reality in science education is its ability to visualize abstract concepts. For example, traditional presentations of 2-D orbitals as point distribution functions and contour surfaces are sometimes simplified. The viewer has difficulties visualizing the true nature of the electron cloud, especially how diffuse or dense it is actually in different regions of the atom. 3-D representations with the possibility of interactivity and navigation through the models have a great potential to increase the effectiveness of educational simulations.

## 3. The "Virtual Water" environment

We have developed the software "Virtual Water", a virtual environment to support the learning of some concepts of Physics and Chemistry by students at the final year of high school or at first year of university. Our virtual environment is centered in the microscopic structure of water and, among others subjects (such as phases of matter and phase transitions), allows to explore atomic and molecular orbitals.

For model development and optimisation we used the commercial software packages *Mathcad* and *3-D Studio Max*. Concerning the definition and creation of the virtual scenarios *WorldToolkit* (from Sense8) was employed.

The minimal hardware requirements for "Virtual Water" are a Pentium III processor, 128 MB of RAM, 150 MB of free hard disc, graphics board accelerator, and Microsoft Windows NT 4.0 or higher.

We proceed describing our methodology in our study. After, we present a short characterization of atomic orbitals sceneries of our virtual environment. Following, we present the research question we have asked to the students before and after software exploration together with some representative answers. Finally we summarize our results and give a selection of free comments made by students.

## 4. Methodology

### 4.1. Objectives

With "Virtual Water" we studied the effect of 3-D interactive simulations on students' visualization of atomic orbitals of hydrogen. For analysing the utility of our program, we have compared the students' answers before and after software use and have tried to find correlations between conceptual comprehension and software use.

### 4.2. Variables and instruments

Our dependent variable is the level of conceptual comprehension on atomic orbitals, while our independent variable was the use of 3-D interactive computer simulations.

The observations of student's attitudes and interviews are the adequate methods in the descriptive studies like the present one [17]. To detect differences between conceptual comprehension without and with software visualization oral answers given by the students were analysed (we video taped students' interviews).

### 4.3. Sample

Our study involved 20 first year students attending Physics, Chemistry, Industrial Chemistry, Physics Engineering and Civil Engineering courses at the University of Coimbra, Portugal. Atomic orbitals had been taught at an introductory level in their courses (they belong to the "General Chemistry" syllabus).

## 5. Results and discussion

Our computer scenarios, which allow for some control by the user, were shown to the students to enhance a deeper understanding of atomics orbitals of hydrogen. The chosen set of scenarios focused on the *1s*, *2s*, *2p*, *3s*, *3p* and *3d* atomic orbitals (Figure 1). In all this scenarios it is possible to rotate the orbitals, choosing different aspects of electron densities, and to experiment diverse cut plans.

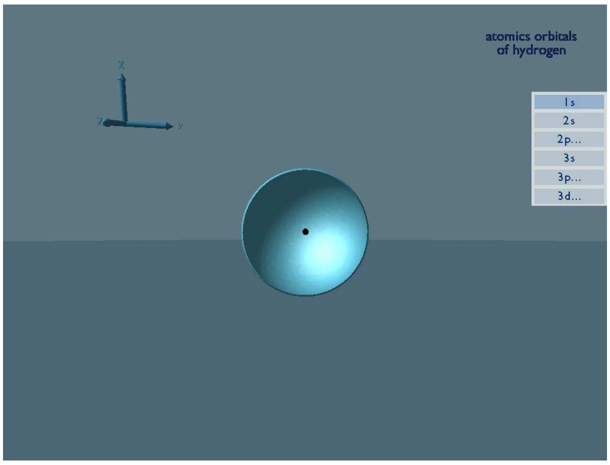
Our research question was: "*how do you conceive electrons in an atom?* Students were prompted to answer the question, before and after seeing "Virtual Water".

The following ideas give an overview of the common conceptions that occurred most often before software use:

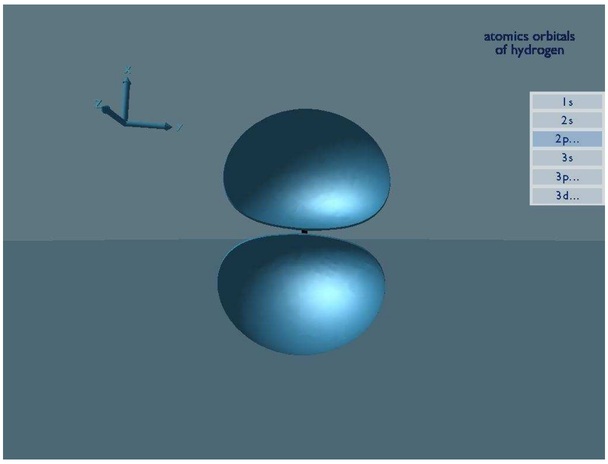
a) Bohr's atomic model (circular orbit). Conceptions of electrons which fly around the nucleus with high speed in prescribed orbits.
b) Charge. Students often explain the properties of charges incorrectly. The charges of both the proton

and the electron cause a distance between the two particles. Students normally assemble a suitable conception from single elements knowledge.

c) Shell. Conception of a firm shell on which the electrons are fixed or move.




a)

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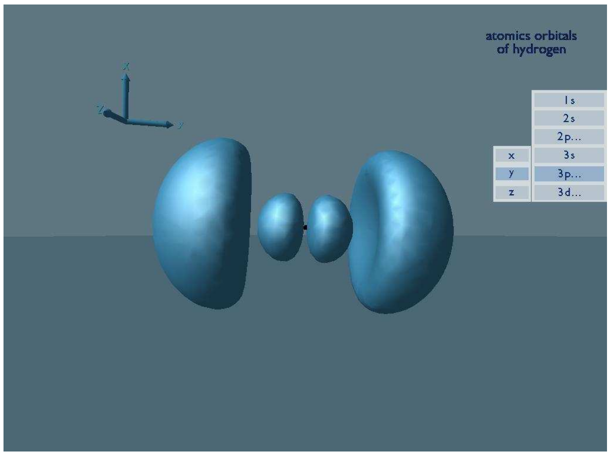


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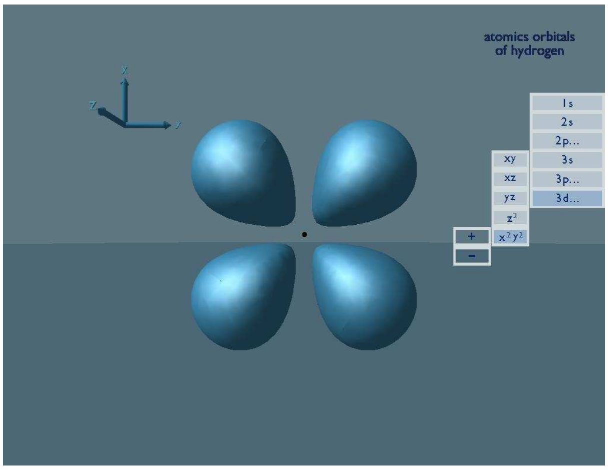


d)

Figure 1. Atomic orbitals of hydrogen being shown the following orbitals: a) 1s; b) $2p_x$; c) $3p_y$; d) $3d_{x^2 y^2}$. The dark point in the centre represents the nucleus of the hydrogen atom. For each orbital it is possible to choose different aspects of electron densities. Figures a) and b) represent models that are cute along the x axis showing the interior of the orbital.

We have made a descriptive statistics of the students' conceptions. In order to enable quantitative comparisons, students' conceptions were considered to lie on an ordinal scale. The array of variable classification ranged from 1 (dead wrong) to 5 (completely right).

Figure 2 shows the boxplots concerning the comprehension of orbitals without software use and after computer visualization. As we can see, the results with software are a little better (we found more correct answers). After software the mean score is 3.55, with a 0.94 standard deviation, while for without software the mean score is 2.10, with a 1.25 standard deviation.

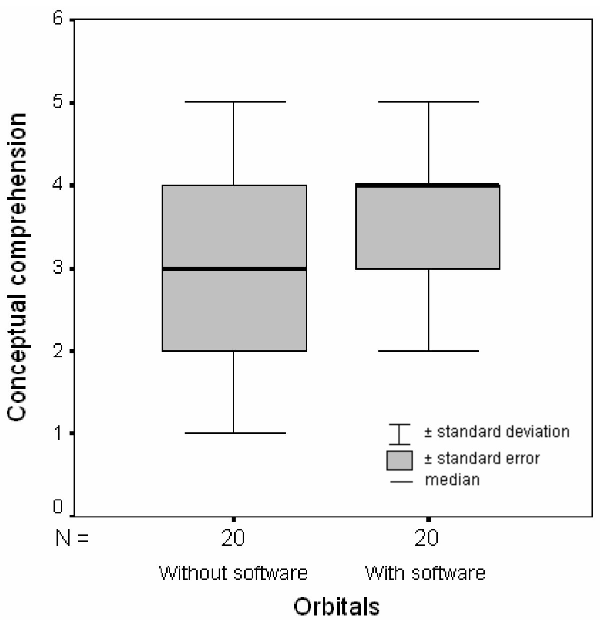


**Figure 2. Boxplots for conceptual comprehension without and with software concerning orbitals.**

Using the Spearman test (at a confidence level of 5%) we found correlations between conceptual comprehension and the characteristics of computer visualization, like 3-D perception and navigation (Table 1).

**Table 1. Correlations between computer visualization and conceptual comprehension of orbitals.**

| Computer visualization | |
|---|---|
| 3-D perception | Navigation |
| 0.560 ($p<0.05$) | 0.459 ($p<0.05$) |

Some other statistical results have been described elsewhere [18].

## 6. Conclusions

We may summarize our conclusions by saying that graphical 3-D visualization tools are useful to increase students understanding of atomic orbitals overcoming their previous misconceptions. The most important characteristics which contributed to students' conceptual comprehension were 3-D perception and navigation.

One of the values of virtual reality is its ability to give substance to abstract concepts. We think that this value was demonstrated in our “Virtual Water” project. Students exposed to our computer environment were in general very enthusiastic. In response to free format questions they wrote that "t*his experience will stay in memory much longer than any notes or lectures*" and "*it is easier to understand things when you can visualize them*".

## 7. Acknowledgements

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