

Students' Visualization and Conceptual Understanding of Atomic Orbitals Using a Virtual Environment

Jorge Trindade^{1,2}

¹ High School for Technology and Management
Polytechnic Institute of Guarda
P-6301-559 Guarda, Portugal
jtrindade@ipg.pt

Carlos Fiolhais²

² Centre for Computational Physics and
Physics Department, University of Coimbra
P-3004-516 Coimbra, Portugal
tcarlos@teor.fis.uc.pt

Abstract

In order to study various aspects of students' 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 or first-year university levels. It focuses on the microscopic structure of water and explores, among others, concepts related to atomic and molecular orbitals.

To evaluate that software, we have made a qualitative study with 20 first-year students of Science and Engineering courses at the University of Coimbra, Portugal. Having been 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 our virtual environment.

1. Introduction

Various authors [1] have defended the regular use of computer simulation and visualization in Physics and Chemistry teaching. They argue that students should be given an active role in using these tools [2]. In particular, there has been an increasing interest in students' misconceptions and difficulties in understanding basic quantum mechanics [3].

While there is a larger number of educational studies which deal with students' conceptions of a specific set of topics at different curricular levels, there are few attempts to probe how students' understanding of core topics change with the use of new visual pedagogical means.

Since students are now much more exposed at an early stage to computer-generated materials, sophisticated graphical representations are required in schools. The presentation of quantum mechanics material has changed over the last years. Recent examples of course materials,

including textbooks and software, allow students to visualize quantum abstract concepts, such as atomic or molecular orbitals.

Modern developments in visualization and computer technologies have created new possibilities in Physics and Chemistry Education for viewing 3-D objects. One of the most promising advanced learning environments for science education is virtual reality.

Virtual reality can indeed be exploited in science education for visualizing abstract concepts. For example, traditional presentations of 2-D orbitals are of course simplified. 3-D representations, with the possibility of interactivity and navigation through the models, have a great potential to increase students' understanding.

Therefore, knowledge of students' visualizations skills, in particular 3-D perception, has become important for testing the effectiveness of such new materials. We give here a contribution to the on-going research on the use of computer-generated 3-D models in science education.

2. The “Virtual Water” environment

We have developed the software “Virtual Water”, a virtual environment to support the learning of Physics and Chemistry by students at the final year of high school or at first-year of university. Our virtual environment deals with the microscopic structure of water and, among others subjects (namely phases of matter and phase transitions), allows to explore atomic and molecular orbitals.

The chosen set of scenarios focused on the $1s$, $2s$, $2p$, $3s$, $3p$ and $3d$ orbitals of the hydrogen atom. In contrast with other software, students may not only visualize the orbitals, but rotate it, select different electronic density surfaces and experiment diverse cut plans (Figure 1). Our computer scenarios were shown to students in order to enhance their understanding of atomic orbitals.

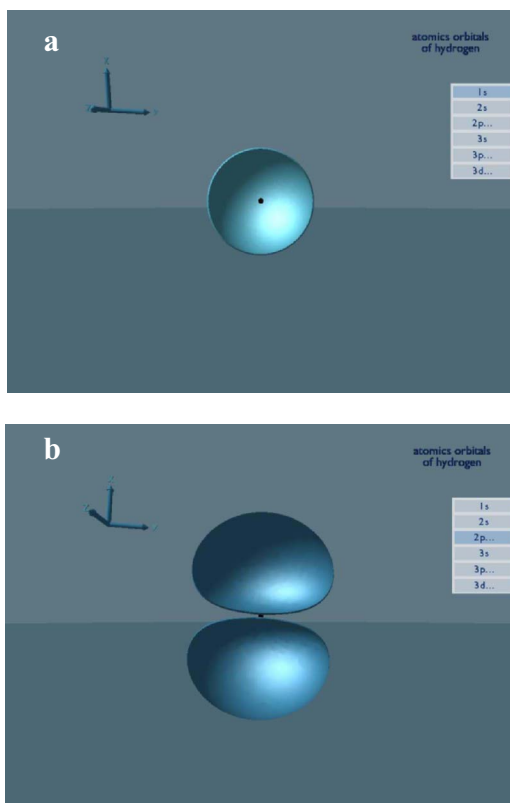


Figure 1. Isoprobabilistic surfaces of atomic orbitals of hydrogen. The following orbitals are shown: a) $1s$; b) $2p_x$. The dark point at the centre represents the nucleus of the hydrogen atom (proton). For each orbital the viewer may choose different views of electron densities. Figures a) and b) represent models that are cut along the xy plane showing the interior of the orbital.

3. Results

With “Virtual Water” we studied the effect of 3-D simulations on students’ perception of atomic orbitals of hydrogen. For analysing the utility of our program, we have compared answers given by a sample of students before and after software use and have tried to find correlations between conceptual comprehension and software characteristics.

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 [4]), but the visual resources have been restricted to pictures.

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”.

We have made a descriptive statistics of the students’ conceptions. The results after software use are somewhat better (we found more correct answers) and we found correlations between conceptual comprehension and some characteristics of computer visualization, like 3-D perception and navigation. Detailed results are described in [5].

4. Conclusions

Graphical 3-D visualization tools seem to increase students’ understanding of atomic orbitals. They contribute to overcome, at least partially, their previous misconceptions. In particular, the idea that electrons move in 3-D space around the nucleus, being their presence more probable in some region than in others, was more interiorised.

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 explored our computer environment with enthusiasm. In response to the format questions one of the students wrote: “*it is easier to understand things when you can see them*”. Since this exploratory study gives positive indications, we intend in the future to incorporate this style of materials in normal classes.

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