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Visualizing Atomic Orbitals Using Second Life

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Abstract

We demonstrate the usefulness of Second Life as a platform for enlivening major concepts in chemistry education. These concepts include absorption spectra, selection rules, quantum numbers, and atomic orbital shapes. We have built several exhibits in Second Life which provide 3-dimensional interactivity for each of those areas: an interactive experiment showing the absorption spectrum of hydrogen, an interactive model of selection rules showing allowed and forbidden transitions for each state, a 3-dimensional grid of orbitals showing the constraints on the values of quantum numbers, and a large-scale interactive orbital display allowing the user to choose and rotate to-scale atomic orbitals based on quantum numbers.

Keywords: virtual worlds; physical chemistry; hydrogen; atomic orbitals.

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Atomic orbitals has been identified as an area of chemistry education needing significant improvement due to student comprehension difficulties (see for example, *1, 2, 3*). Standard software tools, such as Gnuplot (*4*), have been employed to visualize some concepts of orbitals. While these tools do provide a way to view 3-dimensional objects, they lack another important element -- interactivity. Trindade, et al (*5*), using a desktop application of their own creation, have presented some encouraging evidence that using computer-based tools to present interactive 3-dimensional representations of atomic orbitals can "increase student's understanding of atomic orbitals overcoming, at least partially, previous misconceptions." Second Life offers a platform for relatively simple development of complex 3-dimensional, interactive objects, without the need for engaging in application programming. Virtual environments such as Second Life have also been shown to provide an element of presence, which is reported to contribute to more positive student learning outcomes (*6*). Second Life is increasingly being used for education and not just for chemistry (see for example, *7*), with three clear benefits, whatever the discipline: Visualization, Immersion (Presence) and Collaboration.

We have used Second Life as a platform to enliven atomic orbitals and related concepts by creating several interactive exhibits. These exhibits will engage a chemistry student in four basic topics from hydrogen energy levels and atomic orbitals education: absorption spectra, selection rules, quantum numbers, and atomic orbital shapes and relative sizes. Our works are examples of the kind of 3-dimensional interactivity available within Second Life. The exhibits constructed include an interactive experiment showing the absorption spectrum of hydrogen (Figure 1), an interactive model of selection rules showing allowed and forbidden transitions for each eigenstate (Figure 2), a 3-dimensional grid of orbitals showing the constraints on the values of quantum numbers and the relative sizes of atomic orbitals (Figure 3), and a large-scale interactive orbital display allowing the user to choose and rotate to-scale atomic orbitals based on quantum numbers (Figure 4). These exhibits are also freely available for others to customize and improve.

In this paper, we will first briefly discuss our method for creating the atomic orbital shapes within Second Life. Then we will give a detailed presentation of each of the four exhibits. Finally, some concluding remarks will be offered.

Orbital Shapes

Second Life allows for the construction of objects by simple primitive objects, such as a sphere or box. It also allows for sculpted-prim maps which specify custom details about the object's shape. With these tools, exact orbital representations would be difficult to dynamically create within Second Life in the same way as other computer-generated images are usually created[2]. Instead, we created several sculpted-prim maps of the lobes of orbitals based upon the roots of a ninety-percent integral of the square of the radial function. These root values served to mark radial boundaries for the orbitals. The lobes created from the prim maps were then re-sized

and positioned according to this data. Once the lobes were accurately positioned, colored to show positive and negative wavefunction values, and textured, we linked them together to form to-scale 3-dimensional orbitals in Second Life.

Exhibits

Some of the important concepts in hydrogen energy levels and atomic orbitals education are those of energy level transitions and spectra. We have provided a demonstration of the Balmer Series by passing white light through a container of hydrogen orbitals that absorb light and visibly jump to higher energy states, and then through a prism. The resulting absorption spectrum is cast onto a screen, which includes a description of the spectrum. The system can be turned on or off by touching the light source. When the light source is off, the light and the spectrum disappear; when on, the light and the spectrum are visible. The user can also cause more hydrogen orbitals to appear inside the container by clicking on it, and photons of appropriate color (wavelength) can be observed being emitted from the orbitals as they decay back to lower energy states. There is a slide nearby which briefly explains spectra and includes a link to a web page having more information about the topic.
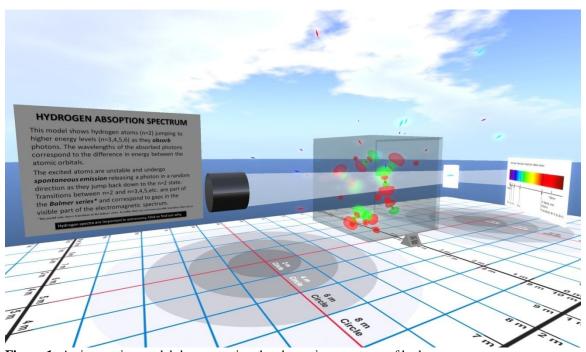

Figure 1: An interactive model demonstrating the absorption spectrum of hydrogen.

Another exhibit demonstrates valid transitions between states as prescribed by selection rules. It has a box for each orbital. Each box shows the quantum triplet associated with that orbital. The boxes are arranged with n varying with height, l with depth, and m from side to side. This arrangement is similar to the stereoscopic depiction presented by Graham *(8)*. The user selects a box as the initial state by touching it. The exhibit then highlights the states which mark allowable transitions. A slide explains the demonstration and provides a link to a web page with more detailed information about selection rules.
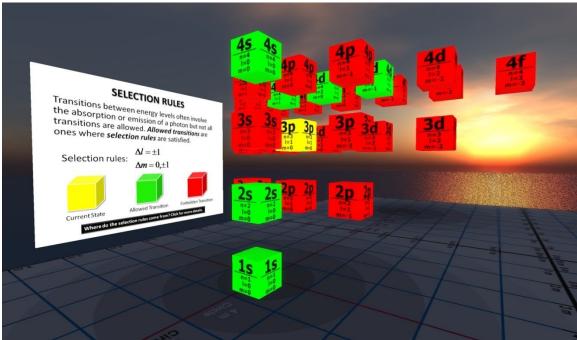
Figure 2: An interactive model demonstrating selection rules.

Another exhibit shows all of the orbitals from n = 1 to n = 4, inclusive. These orbitals are arranged similarly to the boxes in the selection rules exhibit. The exhibit is a visual display showing the constraints on the values of quantum numbers and their relationship to orbital shape and size; however, the visual experience is enlivened by the ability to move around (and within) the exhibit to get different views of the orbitals.
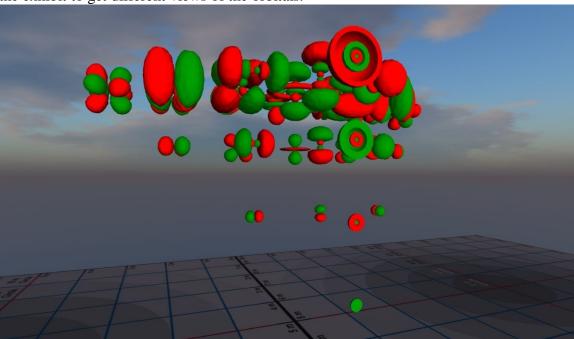

Figure 3: A 3-dimension model of to-scale atomic orbitals arranged by quantum numbers.

Lastly, we have an exhibit which allows the user to manipulate and display orbitals using a control panel. To begin with, the control panel has a button which gives the user usage instructions when pressed. The panel also has a set of buttons to control the quantum numbers n, l, and m and thereby control which orbital is displayed. For each of the quantum numbers, there is an up button and a down button. Pressing the up button will increase the value of the associated quantum number, and pressing the down button will have the opposite effect. These buttons follow the rules of quantum number combinations. For example, suppose that the current quantum number selections are $n = 2$, $l = 1$, and $m = +1$. Then, the l and m up buttons are faded, and pressing the up button for m specifically results in the receipt of a message: "The absolute value of m cannot be greater than l." Thus, a student could develop a better grasp of the rules governing quantum number combinations simply by "playing" with these buttons and reading the messages.
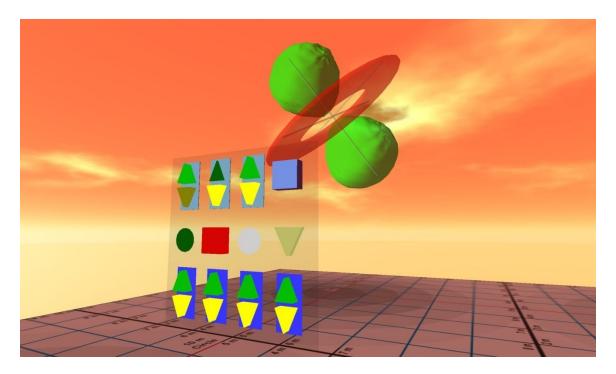

Figure 4: An interactive model that allows for the selection and rotation of all orbitals up to and including n=4.

Along with the display of the orbital is the name of the orbital (not visible in Figure 4). Furthermore, the control panel has a button for switching to a solid cutaway mode for the s orbitals, so that the student can more readily see the concentric spheres. The panel also has a button for rotating the orbital. The rotation can be controlled by altering the x, y, and z values which determine the axis of rotation. The speed can also be specified in radians/second. Additionally, each orbital's Cartesian axes are labeled so that the student can more readily see the correlation between the name of the orbital and its orientation with respect to those axes.

Conclusion

The exhibits that we have created provide examples of how Second Life can be used to strengthen and enliven chemistry courses in the area of atomic orbitals. Nevertheless, a true appreciation of our work can only be attained in-world. The exhibits are displayed on Nature's Elucian Island[3]. They are provided for anyone to use them as they are; additionally, the exhibits have been released to the general public via Xstreet SL. Thus, we present this work as more than a set of exhibits to use; we present them also as a set of tools for individual use and adaptation. For example, a chemistry educator could set these up in a personal lab area in Second Life, with slide presentations, and conduct one or more classes within Second Life. Additionally, the original scripts and objects themselves can be modified to include other desired features.

Notes

1. The Orbitron provides a resource of 3-d orbital images. See
http://winter.group.shef.ac.uk/orbitron.

2. SLurl to our virtual lab housing the exhibits:
http://slurl.com/secondlife/Elucian%20Islands/26/50/353

3. You may obtain full permissions versions of all our exhibits here:

http://www.xstreetsl.com/modules.php?name=Marketplace&MerchantID=180472

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