Do-It-Yourself: 3D Models of Electronic Orbitals through 3D Printing

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Abstract:
Everything in the entire universe is made up of atoms, which can be broken down into three subatomic particles: protons, neutrons, and electrons. In quantum mechanics, mathematical shape functions called electronic orbitals model electron behavior. In other words, mathematical shapes, plotted in spherical coordinates, represent the likelihood of finding an electron at a given location in an atom. Beginning level science students often find difficulty in visualizing 3-dimensional models for electron orbitals, especially when most representations are provided in 2-dimensions. Our research has been in effort to create tangible, 3-dimensional representations of electron orbitals. Creation of the models requires a program capable of graphing the electron orbitals in 3D and exporting the graph as a stereolithography (.stl) file. The 3D printer used requires the use of .stl files to interpret graphical data. The free web-based applet, 3D Calc Plotter, was selected for this project. After a virtual model of the electron orbital was rendered, the .stl file was exported to the 3D printer and used to create the physical models of electron orbitals.

Introduction:
In reality, electrons exhibit a more complex, matter-wave duality and occupy a finite, three-dimensional space around a nucleus known as an orbital. These electron orbitals are modeled by the Schrödinger Wave Equation: \( \psi(x, y, z) \). These models are often difficult for students to conceptualize if drawn on a 2-D textbook page.

Schrödinger Wave Equation:

\[
\psi(r) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} e^{-r^2} dr
\]

Determines the appearance of the orbital.

\[
\psi^2 = R(r)^2 \times Y(\theta, \phi)^2
\]

Radial Function \( R(\rho) \):
Determines orbital size.

\[
\psi \cdot \mathbf{\hat{r}}
\]

Angular Function \( Y(\theta, \phi) \):
Determines orbital shape.

Example quantum mechanical wave equation for the \( 2p_x \) orbital:

\[
\psi = (3cos^2(\theta - 1))^2
\]

Modeling Wave Equations:

Advantages of 3D Calc Plotter:

- Able to export models as stereolithography (.stl) files, or "3D printer files"
- "3D printer files"
- Allows graphing in spherical coordinates
- Support structures
- Freeware

3-D Printing Process:

All matter in the universe is made up of atoms, submicroscopic particles with three constituent particles:
- Protons (positive charge)
- Neutrons (neutral)
- Electrons (negative charge)

In 3D printing, the 3D printer generates an object based on the digital model provided. The model is sliced into layers and each layer is built up using a 3D printing technique. In this case, the 3D printer was used to create the physical models of electron orbitals.

Final Product: Atomic Orbitals

Representative atomic orbitals (from left): a 2p combo, 2s cross-section, a 4p, a 4d, and a 4f.

Final Product: Hybrid Orbitals

Representative hybrid orbitals (from left): 2sp combo, 2sp d combo, 2sp f, 2p6, and 2p9 orbitals.

Hybrid Orbitals:
Covalently bonded atoms within molecules must share electrons, thus the atoms must “share” the orbitals. In preparation for this sharing, atoms transform their atomic orbitals my mixing them together to form hybrid orbitals. This mixing helps the atom achieve an optimal bonding arrangement.

Modeling Hybrid Orbitals:

- Hybrid orbitals are generated by linear combination of individual atomic orbital wave equations.
- This hybrid orbital is the sum of a 2s+2p orbital.

Final Product: Hybrid Orbitals

A 2sp hybrid orbital generated in 3D Calc Plotter.

The 2sp hybrid orbital wave equation inserted in the 3D Calc Plotter 3D Implicit Function toolbar.

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Reference:

1. https://inside.sparkfun.com/assets/3/6/1/2/2135a57df7fe490156e000000.png

Conclusion:

After extensive research of 3D graphing programs, 3D Calc Plotter offered the best combination of cost, mathematical capability, and 3D printing compatibility.

- Nodes represented an engineering challenge as the model needed to be connected at these points via structural support.
- Orbitals have proved successful as pedagogical tools in introductory chemistry courses.

Future Goals:

- Develop working supply of models for continued use in the classroom.
- Explore the development of further quantum mechanical models for behavior of electrons in atoms and molecules.

References:

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