A student-generated less-familiar atomic orbitals (*l* = 4–10) representation using simple and real-time visualization software

La representación de los orbitales atómicos menos conocidos (*l* = 4-10) usando simple software de visualización

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Abstract

Hydrogen atomic orbitals generally introduced to chemistry students are restricted to s (l = 0), p (l = 1), d (l = 2), f (l = 3) orbitals. This way makes student wonder about what the post-f orbitals look like. The literature provides very little information on this. In this situation, teachers usually simply represent orbitals in Power Point slides or transparencies without involving students in constructing an orbital from its original equation. This work provides a simple way to real-time plotting of 105 lesser known atomic orbitals (l = 4–10) for learning projects in the classroom. Constructing orbitals on their own project allows students to become familiar with less well known orbital characteristics and their related equations.

Key words: computer-based learning, atomic orbital, physical chemistry

Resumen

Orbitales atómicos del hidrógeno introducidos generalmente a estudiantes de química están restringidos a s (l = 0), p (l = 1), d (l = 2), f (l = 3) orbitales. De esta manera hace que el estudiante pregunte acerca de lo que parecen los orbitarios después de f. La literatura proporciona muy poca información sobre esto. En esta situación, los profesores generalmente, simplemente representan orbitarios en diapositivas o transparencias sin que los estudiantes participen en la construcción de un orbital de la ecuación original. Este trabajo proporciona una forma sencilla de trazar en tiempo real de 105 orbitales atómicas menos conocidas (l = 4-10) para el aprendizaje de proyectos en el aula. Construir orbitales en su propio proyecto permite a los estudiantes familiarizarse con las características de orbitales y sus ecuaciones relacionadas.

Palabras clave: aprendizaje asistido por computadora, orbital atómico, físicoquímica

INTRODUCTION

One of the biggest challenge for chemistry teachers is how to teach an abstract concepts in chemistry to become a physically interpretable concept which has direct application in real life. Generally, teachers worry when teaching concepts such as atomic structure which have no direct link to real life and require spatial imagination (Finley et al., 1982; Tsaparlis, 1997; Niaz, 2002; Park & Light, 2009). Nevertheless, those topics should be taught because understanding of atomic structure has consequences for the way students understand chemistry (Taber, 2003).

The Indonesian ministry for education enacts concept mastery on atomic structure topics as a mandatoried competency standard for secondary chemistry students. The competency standard requires that the student is able to analyze the historical background of atomic model, the atomic structure based on Böhr and quantum mechanics theory, and the relationship between electron configuration and orbital diagram to determine the location of elements in the periodic table and periodic properties of elements (Indonesian Curriculum Standard for Secondary Education, 2013). However, there are several views on whether the quantum chemistry concepts is suitable for secondary and undergraduate students, although most of them agreed to teach it with some strategies than leave out (Tsaparlis, 1997; Budde et al., 2002; Tsaparlis & Papaphotis, 2002; Park & Light, 2009). In this case, even if teaching modern quantum chemistry concepts shows many barriers, they should be introduced, and they are necessary if it really needed, with great care (Tsaparlis, 1997; Tsaparlis & Papaphotis, 2002). For example, Polydoropoulos (1974) suggest the careful introduction of a mathematical function describing an electron in an atom or molecule and pictorial models must be built onto the mathematics to turn it into a useful intuitive tool (Tsaparlis & Papaphotis, 2002). Therefore, learning atomic structure should be designed more interactive, educative, and realistic so that students appreciate the importance of this topic.

Nowadays, teaching atomic structure theory is focused on Schrodingers' overviews which is the most accepted electronic structure theory. In principle, this theory applies Schrodingers' wave equation to explain entire electronic properties of molecules, and should be capable of describing all aspects of bonding. Moreover, learning modern atomic structure should introduce the ideas of an "orbital" as a core concept that represents the most probable volume in which an electron will be found. Teaching about orbitals is restricted to only *s, p, d, f* (*l* = 0–3) orbitals since this is sufficient to cover the electronic structure (ground state) of all elements in the Periodic Table. There is very little literature provided concerning the representation of post-*f* orbitals or help for teachers to deliver orbital concepts interactively. On this topic, physical chemistry teachers usually use traditional teaching strategies without allowing students to construct orbitals in their own projects. Those conditions potentially raise some disadvantages such as: (a) wrong interpretation that orbitals only exist for *l* = 0–3, (b) students'will not understand about how orbitals is constructed, post-*f* orbitals' characteristics, and "the components" determined orbital shapes and orientations. Thus, students' personal activities in constructing less familiar' orbitals (*l* > 3) could be quite important.

Students' projects in constructing orbitals can be effectively facilitated by applying graphical visualization tools. Producing orbital representation from its corresponding mathematical equation is believed to encourage students to understand equation-graph relationship and characteristics of the produced graph. Some researchers have reported the functionalities of mathematical softwares like Matlab (Shechter, 2016), Matcad (Ellison, 2004), Mathematica (Cooper & Casanova, 1991), Maple (Stewart, 2013), to visualize orbital. However, these applications are not suitable for beginners because they require special coding skills. Chung (2013) suggested a free-distributed software named Winplot (Parris, 2012) that is usable for beginners (without complicated scripting) and has applied this software to plot the shape of *s, p, d* atomic orbitals. Our previous study (Saputra, 2015) has also used this software to visualize three dimensional hybrid atomic orbitals. This recent study provides a strategy to create 105 lesser known atomic orbitals (*l* = 4-10) using Winplot. Constructing less familiar atomic orbitals in a student's own project is expected to enhance the student's understanding about post-*f* orbitals and actively participate in learning modern atomic structure.

RESULT AND DISCUSSION

Deriving the wave equation

The Schrodinger wave function as generally known consists of radial *R* (*r*) and angular *Y* (*θ,ϕ*) components. By referring to many standard physical chemistry textbooks (McQuarrie, 1983; Atkins & Paula, 2010; Mortimer, 2008), anyone can understand that orbital shapes and orientations is only determined by the angular parts, whereas radial parts determines the size of orbital. The general equation for angular parts is shown in equation 1.

$$Y_{(\theta, \varphi)} = \left(\frac{2l+1}{4\pi} \frac{(l-|m|)!}{(l+|m|)!} \right)^{1/2} P_l^{|m|}(\cos\theta) e^{im\phi}$$

where $P_l^{|m|} = \frac{1}{2^l l!} \left(1-x^2\right)^{\frac{|m|}{2}} \frac{d^{1+m}}{d^{l+m}x}\left(x^2-1\right)^l$ is associated Legendre function

with *l* and *m* is azimuthal and magnetic quantum number, respectively (McQuarrie, 1983). The complete wave function and its corresponding winplot code can be provided in the Supporting Information (Please contact authors by email).

Visualizing non-famous orbitals

By simply converting the angular wave equations in table 1 to Winplot code as described by Chung (2013), one can visualize many types of less familiar atomic orbital representation. As example, representation of orbital for $l = 4$ is presented in figure 1.

$l = 4$
$m = 0$

$l = 4$
$m = \pm 1$

$l = 4$
$m = \pm 2$

$l = 4$
$m = \pm 3$

$l = 4$
$m = \pm 4$
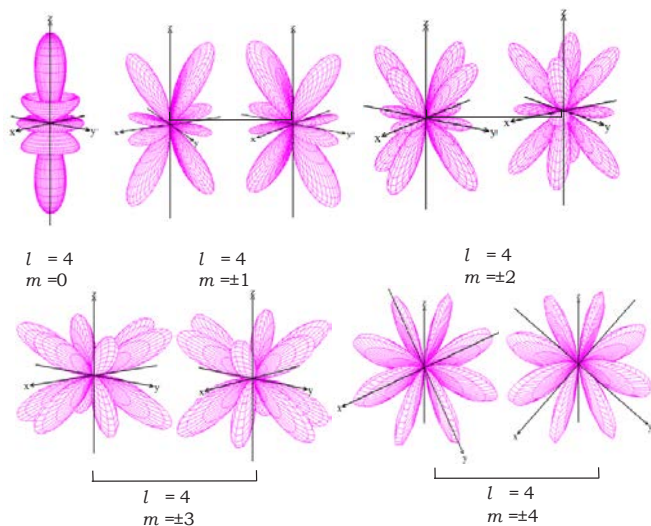
CONCLUSIONS

A large set of less familiar atomic orbitals has been successfully generated by students using simple Winplot software. Applying Winplot makes students project to visualize orbital become simple and possible. Then, this powerful software is highly recommended to be used in teaching atomic structure in schools or universities.

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BIBLIOGRAPHY

Atkins, P. W., Paula, J. D., *Physical Chemistry*, 9th ed., W. H. Freeman: Madison Evenue, NY, 2010, p. 374 −377.

Budde, M., Niedderer, H., Scott, P., Leach, J., 'Electronium': a quantum atomic teaching model, *Physics Education*, **37**, [3], 197–203 , 2002.

Chung, W. C., Three-Dimensional Atomic Orbital Plots in the Classroom Using Winplot, *Journal of Chemical Education*, **90**, [8], 1090-1092, 2013.

Cooper, R., Casanova, J., Two-Dimensional Atomic and Molecular Orbital Displays using Mathematica, *Journal of Chemical Education*, **68**, [6], 487−488, 1991.

Ellison, sp³dⁿ Hybrid Orbitals and Molecular Geometry, *Journal of Chemical Education*, **81**, [10], 1534, 2004.

Finley, F.N.; Stewart, J.; Yarroch, W.L., Teachers' perceptions of important and difficult science content, *Science Education*, **66**, [4], 531-538, 1982.

Indonesian Curriculum Standard for Secondary Education, Content Standard of Chemistry for Secondary School, General Board of Elementary and Secondary Education, Jakarta, Indonesia, 2013.

McQuarrie, D. A., Quantum Chemistry, *University Science Books*, Sausalito, CA, 1983, p. 398 − 407.

Mortimer, R. G., *Physical Chemistry*, 3rd ed., Elsevier Academic Press: Burlington, MA, 2008, p. 853 - 855.

Niaz, M.; Aguilera, D.; Maza, A.; Leindo, G., Arguments, contradictions, resistances, and conceptual change in students' understanding of atomic structure, *Science Education*, **86**, [4], 505-525, 2002.

Park, E.J., Light, G., Indentifying atomic structure as a threshold concept: students mental models and troublesomeness, *International Journal of Science Education*, **31**, [2], 233-258, 2009.

Parris, R., Winplot Home Page, http://math.exeter.edu/rparris/winplot.html (accessed Jun 2016).

Shechter, E., Matlab Home Page, http://www.mathworks.com/matlabcentral/ileexchange/44604-plot-hydrogen-atom-molecular-orbital (accessed Jun 2016).

Saputra, A., Canaval, L.R., Sunyono, Fadiawati, N., Diawati, C., Setyorini, M., Kadaritna, N., Kadaryanto, B., Visualizing Three-Dimensional Hybrid Atomic Orbitals Using Winplot: An Application for Student Self– Instruction, *Journal of Chemical Education*, **92**, [9], 1557-1558, 2015.

Stewart, B., Hylton, D. J., Ravi, N., Using Maple to Visualize Atomic Orbitals, *Proceedings of The National Conference On Undergraduate Research (NCUR), University of Wisconsin La Crosse,* 11-13 Apr 2013, University of Wisconsin, 2013, p. 303-308.

Taber, K.S., The atom in the chemistry curriculum: fundamental concept, teaching model or epistemological obstacle?, *Foundations of Chemistry*, **5**, [1], 43–84, 2003.

Tsaparlis, G., Atomic orbitals, molecular orbitals, and related concepts: conceptual difficulties among chemistry students, *Research in Science Education*, **27**, [2], 271-287, 1997.

Tsaparlis, G., Papaphotis, G., *Quantum-chemical concepts: are they suitable for secondary students?, Chemistry Education:* Research And Practice In Europe, 3, [2], 129–144, 2002.

Books review

Eric R Scerri. A TALE OF SEVEN SCIENTISTS AND A NEW PHILOSOPHY OF SCIENCE. Published by Oxford University Press, 2016. ISBN: 9780190232993
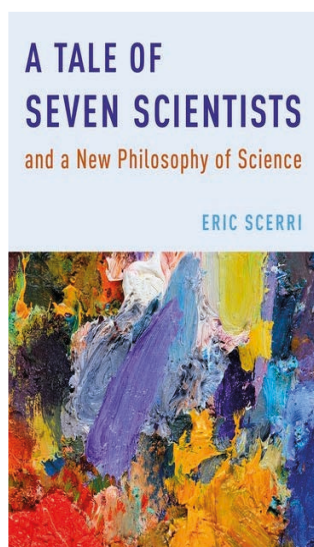
This is an intriguing book that provides an extensive source of information about seven little-known chemists and their contribution the development of chemical ideas. It also pictures the nature of scientific development in ways that challenge our more usual views. The author perceives the progress of science to be much more an 'evolution to fit the environment' than a closer approach to the truth, snd ascribes value to 'wrong theories'.

In the preface to the book there are two perceptive forewords by Peter Atkins and by James Marcum and also, a fairly extensive autobiographical summary of the author's own professional growth as a chemist and philosopher of chemistry. This last provides a valuable insight for the reader into the possible sources of the 'new philosophy of science' that is presaged in the title of the book. Such a section should probably be mandatory in any publication in which new, and possibly controversial, ideas are being propounded.

The 'seven scientists' in the title are each provided a chapter within the main text and their names are John Nicholson; Anton Van den Broek; Richard Abegg; Charles Bury; John D Main Smith; Edmund Stoner and Charles Janet. The main chapter headings are reproduced below, together with a few comments in *italics*.

Chapter 1. Introduction: Intermediate historical figures & how can 'wrong theories' lead to scientific progress?

Chapter 2. The intriguing case of John Nicholson. *This provides examples of some very impressive results from a theory that turned out to have no foundations. It is argued that this work contributed significantly to the conclusions of Niels Bohr – despite being wrong. There seems to be a couple of typographical errors (e.g. in the text, 'c' is given for the speed of light whereas 'a' seem to be used for this within the equations on p16-17), but these are minor faults.*

Chapter 3 Van den Broek and atomic number. *A very good case is made for Van den Broek being the first to recognize the importance of atomic number – rather than atomic weight – in structuring the Periodic Table. I was also fascinated to read that since, within his calculations, hydrogen was anomalous he **omitted** it from his tables!*