

**LEMBAR**  
**HASIL PENILAIAN SEJAWAT SEBIDANG ATAU PEER REVIEW**  
**KARYA ILMIAH : JURNAL ILMIAH INTERNASIONAL**

Judul Jurnal Ilmiah : A Learning Exercise using Simple and Real-Time Visualization TOOL to Counter Misconceptions about Orbitals and Quantum Numbers  
(Artikel) : <http://www.scientiasocialis.lt/jbse/?q=node/516>

Penulis Jurnal Ilmiah : Sunyono, Lisa Tania, Andrian Saputra

Identitas Makalah :

- a. Nama Jurnal : Journal of Baltic Science Education
- b. Nomor/ Volume : Vol. 15, No. 4,
- c. ISSN : 1648-3898
- d. Edisi ( Bulan/Tahun) : 2016
- e. Penerbit : Journal of Baltic Science Education
- f. Jumlah Halaman : pp: 452-463
- g. INDEX / IF : Terindeks Scopus Q2, SJR 0,44

Kategori Publikasi Jurnal Ilmiah :

(beri tanda V pada kategori yang tepat)

- ☒ Jurnal Ilmiah Internasional (Memiliki Faktor Dampak-Thomson Reuters/SJR)
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No	Komponen yang dinilai	Nilai Maksimum Jurnal Ilmiah Internasional :			Nilai yang Diberikan Penilai (NP)
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		<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	
a	Orisinalitas (20%): (Memperlihatkan keaslian dan kebaruan gagasan)	8,00	6,00	4,00	7,5
b	Kedalaman Kajian (40%): (Melakukan analisis, eksplorasi, dan elaborasi terhadap masalah yang dibahas berdasarkan kaidah-kaidah ilmiah yang berlaku dalam penelitian dan pengkajian; mengandung kebenaran ilmiah, ketuntasan kajian, kesistematikan pembahasan, dan didukung dengan pustaka yang relevan)	16,00	12,00	8,00	15
c	Kebermanfaatan (10%): (Memberikan manfaat bagi kemajuan ilmu dan solusi bagi masalah yang dihadapi masyarakat)	4,00	3,00	2,00	4
d	Relevansi karya dengan keahlian (20%) (Memiliki keselarasan antara karya ilmiah dengan penelitian magister/ doktor dan bidang penerapannya)	8,00	6,00	4,00	7,5
e	Kelengkapan unsur Jurnal Ilmiah (10%) (Mencakup prakata, daftar Isi, editor, ISSN, dan kelengkapan lain)	4,00	3,00	2,00	4
Total (100%)		40,00	30,00	20,00	38

Penilaian Kualitatif\*)

Artikel ini mencanbri kesalahan konsep pada konsep orbital dan bilangan kuantum dengan memisali sarkba dengan menggunakan grafik.

Nilai Pengusul = BP x NP = 0,6... X 38..... / 1..... = 22,8

Ket : Bobot Peran (BP) : Sendiri = 1; Ketua = 0,6; Anggota = 0,4 dibagi jumlah anggota

Jambi, ..... 2020  
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a	Orisinalitas (20%): (Memperlihatkan keaslian dan kebaruan gagasan)	8,00	6,00	4,00	7,6
b	Kedalaman Kajian (40%): (Melakukan analisis, eksplorasi, dan elaborasi terhadap masalah yang dibahas berdasarkan kaidah-kaidah ilmiah yang berlaku dalam penelitian dan pengkajian; mengandung kebenaran ilmiah, ketuntasan kajian, kesistematikan pembahasan, dan didukung dengan pustaka yang relevan)	16,00	12,00	8,00	18
c	Kebermanfaatan (10%): (Memberikan manfaat bagi kemajuan ilmu dan solusi bagi masalah yang dihadapi masyarakat)	4,00	3,00	2,00	4,0
d	Relevansi karya dengan keahlian (20%) (Memiliki keselarasan antara karya ilmiah dengan penelitian magister/ doktor dan bidang penugasannya)	8,00	6,00	4,00	7,6
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Total (100%)		40,00	30,00	20,00	38,2

**Penilaian Kualitatif\*)**

Artikel ini telah berhasil meminimalisir miskonsepsi siswa dalam mempelajari konsep orbital dan bilangan kuantum, melalui visualisasi grafik sederhana menggunakan Winplot.

Nilai Pengusul = BP x NP = 0,6 x 38,2 / 1 = 22,92

Ket : Bobot Peran (BP) : Sendiri = 1; Ketua = 0,6; Anggota = 0,4 dibagi jumlah anggota

Solo, 10 Oktober 2020  
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*Sulistyo*

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# LEMBAR

## HASIL PENILAIAN SEJAWAT SEBIDANG ATAU PEER REVIEW

### KARYA ILMIAH : JURNAL ILMIAH INTERNASIONAL

Judul Jurnal Ilmiah

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Total (100%)		40,00	30,00	20,00	38,5

Penilaian Kualitatif\*)

Artikel ini memiliki keaslian dan kebaruan gagasan serta kedalaman kajian yang cukup baik. Selain itu memiliki manfaat bagi kemajuan ilmu dan sangat relevan dengan bidang keahlian penulis. Secara umum artikel/jurnal ini sangat memenuhi kelengkapan unsur jurnal dan berkualitas baik.

Nilai Pengusul = BP x NP = 0,6... X 38,5... = ...23,1

Ket : Bobot Peran (BP) : Sendiri = 1; Ketua = 0,6; Anggota = 0,4 dibagi jumlah anggota

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# A Learning Exercise using Simple and RealTime Visualization TOOL to Counter Misconceptions about Orbitals and Quantum Numbers

*By* Sunyono



JOURNAL  
OF BALTIC  
SCIENCE  
EDUCATION

ISSN 1648-3898

**Abstract.** *Misconception is one of the most widely researched topics in science education, including chemical education. This research aims to apply simple graphical visualization tool named Winplot for a learning exercise activity and explore its potency to counter misconceptions about orbitals and quantum numbers. Misconceptions that were countered in this research are the existence of orbitals in atoms and the relationship of magnetic quantum numbers to orbital orientation.*

*This quasi experimental research using pre-test-post-test control group design was conducted to 43 first-year undergraduate students as control class and 45 as experimental class of chemical education at the University of Lampung. The students' pre-existing concepts were analyzed using a pre-test instrument and explored further using in-depth interview. Then, after implementing a learning exercise activity, the conceptual changes were analyzed using a post-test instrument. The results showed that students in experimental class had significant conceptual changes compared to control class. Applying this computer-based strategy is highly recommended to guide students in understanding chemical concepts, especially the topics of orbitals and quantum numbers.*

**Key words:** *learning exercise, first-year undergraduate, computer-based learning, misconceptions, quantum chemistry.*

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## A LEARNING EXERCISE USING SIMPLE AND REAL- TIME VISUALIZATION TOOL TO COUNTER MISCONCEPTIONS ABOUT ORBITALS AND QUANTUM NUMBERS

**Sunyono Sunyono,  
Lisa Tania,  
Andrian Saputra**

### Introduction

One of the science learning objectives in school is if students can understand and solve many problems occurred in daily life. Therefore, science learning is more focused on the understanding of phenomena that lead to contextual-based teaching and learning. Scientific concepts are contextually introduced to students through phenomena that are generally known in everyday life (Pilot & Bulte, 2006; Gilbert, 2006; Miri et al., 2007; De Jong et al., 2013; Ültay, 2015). However, the experiences of everyday life generate pre-existing concepts about scientific phenomena that can interfere with students understanding of the correct scientific concepts (Taber, 2001; Yip, 2001; Uzuntiryaki & Geban 2005). Incorrect pre-existing concepts lead to persistent misconceptions and cause difficulties in understanding new concepts (Read, 2016). A misconception is a mental representation of a concept that does not correspond to currently held scientific theory. In other words, a misconception can be defined as any concept that differs from the commonly accepted scientific understanding (Nakhleh, 1992). Misconceptions are caused not only by wrong self-interpretation about life phenomena but also by incorrect concepts delivered by teachers or textbooks (Tsaparlis & Papaphotis, 2002; Tsaparlis & Papaphotis, 2009; Kalkanis et al., 2003; Stefani & Tsaparlis, 2009).

Chemistry is a branch of natural science that has many misconceptions in its teaching and learning. Misconceptions in chemical education generally arise because chemistry contains many abstract concepts in addition to complicated calculations. Many students fail to learn chemistry because they do not have a strong understanding of fundamental chemistry concepts that are necessary to construct more advanced ones. In addition, they also do not understand sub-microscopic concepts for explaining the macroscopic world. It is difficult to shift the paradigm of students from a macro to a sub-micro level. They often assume that chemistry is a macro-life science, not a sub-micro one (Johnstone, 1991; Tsaparlis, 1997; Robinson, 2003). Two of the topics





in chemistry that frequently contain misconceptions are orbitals and quantum numbers. Some misconceptions of orbital are that (a) orbitals are trajectories arranged around the nucleus where electrons rotate (Nakiboglu, 2003), (b) an orbital is a fixed energy level where the electron is found (on a Bohr Model) (Müller & Weisner, 2002), and (c) an orbital is a box that can be filled with electrons (Nakiboglu, 2003). Furthermore, misconceptions about quantum numbers, described by Papaphotis & Tsapalis (Papaphotis & Tsapalis, 2008), are that the principal quantum number ( $n$ ) shows the number of shells, the azimuthal quantum number ( $l$ ) shows the number of subshells, the magnetic quantum number ( $m_l$ ) determines the form of the atom in space, and the fourth magnetic quantum number ( $m_s$ ) determines the spin - whether the electrons are found in pairs or alone. These fatal misconceptions indicate that students do not have a comprehensive understanding of orbitals and quantum numbers.

An effective strategy to counter these misconceptions is computer-assisted learning. Computer-assisted chemistry learning is intended to provide more detailed visualizations of chemical processes at a sub-microscopic level. Jones et al. (2005) explain that learning by graphical visualization can significantly help students in understanding the sub-microscopic world. Some studies have been conducted to use computer software to enhance students' understanding of orbitals and quantum numbers (Harvey & Gingold, 2008; Trindade & Fiolhais, 2003; Lang & Kobilynky, 2009; Chung, 2013; Stewart et al., 2013; Chen et al., 2015; Saputra et al., 2015). For example, Lang & Kobilynky (2009) used *Second Life* to visualize atomic orbitals. Furthermore, Stewart et al. (2013) applied the *Maple* program to counter common misconceptions of undergraduate students in General Chemistry courses about atomic orbitals.

#### Problem of Research

Some misconceptions in atomic structure and quantum chemistry learning that commonly occurred are the existence of orbitals and the relationship between orbital shapes and orientations to quantum numbers. Most of chemistry students confused some questions such as (a) do orbitals really exist in atoms, (b) whether orbital shapes and orientations, as commonly known in textbook, are experimental observation or theoretical construction, (c) can the magnetic quantum numbers be freely exchanged for each type of  $p$  and  $d$  orbitals. In this research, a learning exercise using simple and real-time visualization tool was used and explores its potency to counter those misconceptions.

#### Research Focus

A simple and open-source based application named Winplot, has been widely used in the field of educational research. Winplot, which was developed by Richard Parris of the Phillips Exeter Academy, New Hampshire (Shechter, 2016), provides an alternative way to easily plot mathematical equations as useful physical interpretations (Saputra et al., 2015). Some studies have used Winplot to visualize hydrogen atomic orbitals and hybrid orbitals (Chung, 2013; Saputra et al., 2015; Rhile, 2015). This research will explore the use of Winplot in a learning exercise activity to counter several misconceptions about orbitals and quantum numbers. The results of this research can be utilized by educators to overcome chemical misconceptions and encourage the use of ICT for more effective chemical education.

### Methodology of Research

#### General Background of Research

Most of chemistry students feel worries in learning atomic structure and quantum chemistry because involving abstract concepts, complicated equation needs imagination skills. This condition potentially raised misconceptions. This quasi experimental research with pre-test – post-test control group design was intended to identify those misconceptions, especially existence of orbitals and the link between orbital and quantum numbers that generally occurred in the first-year chemistry undergraduate student. Moreover, the effectivity of a learning exercise using Winplot was also analyzed to counter those misconceptions. This treatment was implemented during three weeks (once a week) and in the last week, a post-test was performed for both classes to evaluate the students' concept. All representations of orbital in this paper were visualized by polar coordinate implemented in Winplot, and derived from the square of the angular wave functions by ignored radial distribution function in this derivation. The



ignorance of radial function was addressed to simplify the equation and code, so that usable for students' self-assignment. This ignorance in orbitals' visualization produced inaccurate representation as a limitation of Winplot and proposed visualization in this paper. The usual representation of orbital is an isosurface, a surface of the wave function with a constant value of  $\psi$  or  $\psi^2$  (or  $\psi^*\psi$ ), whereas the radial wave functions are the product of linear and exponential term in distance, which affect isosurface shape (Rhile, 2015). The use of polar graph of the value of the square of the angular wave function in this paper may lead to misrepresented of boundary surface and distance of orbital from the nucleus as graph suggests.

Another way to visualize orbital is the construction of the contour surfaces of the constant value of the whole wave function (Cohen, 1961; Ogryzlo, 1965; Perlmutter-Hayman, 1969; Linnet & Bordass, 1970; Kikuchi & Suzuki, 1985; Peacock-López, 2003). The contour surface will produce a boundary surface as representation of some definite percentage of the total electronic charge and very potential to generate a better visualization (Perlmutter-Hayman, 1969). However, contour lines method which is applied in some mathematical software, such as mathematica, gnuplot, matlab, requires special coding skills. This requirement is very difficult for beginner or first-year undergraduate student to quick and real-time plotting of orbital in the classroom. Therefore, Winplot with all its shortcomings is used in these learning activities.

#### *Sample of Research*

Sample of research was 98 first-year undergraduate students (consisted of 43 students in control and 45 in experimental class) of chemical education at the University of Lampung. This purposively selected sample is expected to have equal pre-existing concepts about orbitals and quantum numbers as learned in their secondary school.

#### *Instrument and Procedures*

Data regarding their pre-existing concepts were collected by a pre-test instrument in form of open-ended questions about the existence of orbitals and the link between orbitals and quantum numbers. In this research, experimental class was applied a learning exercise using Winplot, whereas control class used conventional instruction that did not rely on computer aided graphical renderings. Instructor in the control and experimental class is the same person. Moreover, instructor in the control class is also aware of the students' misconception as instructor in the experimental class. All conditions in control and experimental classes are the same, except the instructional strategy used in learning. To avoid the misconceptions and give the correct concept in control class, the instructor simply used verbal and drew 2D orbitals in whiteboard without involving students to construct orbital by students themselves.

#### *Data Analysis*

The students' responses were categorized into various levels of understanding i.e. true understanding, partial understanding, misconception, and not answered. True understanding is defined as a response that is aligned with all components of the criteria for a correct answer, which was determined by an expert; partial understanding is a response that includes at least one component of the criteria for a correct answer but not all; misconception is a response that includes incorrect information; and not answered is a blank response. Then, the effectivity of these computer visualization activities was measured by comparing the percentage of students at various levels of understanding for each question. In-depth interview was conducted with 10 students who had a misconception to confirm the reason regarding their responses. Data from the interview was analyzed by classified students' responses based on the similarities of those answers and described as explained in the manuscript. Categorization of students' responses into various levels of understanding used in this research is adapted from Nakiboglu (2003). Categorization presented in this manuscript was conducted by authors and then, this marking was followed by triangulation process. Students' responses marked by authors are validated by 1 expert in chemistry and 2 experts in chemical education. Moreover, validation result was discussed in focus group discussion with all lecturers in Peer Group of Chemical Education at University of Lampung. Therefore, validity and reliability of this marking can be justified scientifically.



## Result of Research

Result of this research consisted of two parts. The first part is analysis of students' pre-existing concepts as shown by the distribution of students' level of understanding for each question in pre-test (Table 1). The second part is the percentage of students at misconception after the treatment of a learning exercise as shown by Figure 1.

Table 1 showed students' pre-existing concepts related to some issues in the topic of orbitals and quantum numbers. Data of pre-existing concepts were obtained after analysis of students' answer to 5 questions in a pre-test instrument and categorized into various level of understanding. These questions asked students to do the following:

1. describe the meaning of atomic orbitals
2. clarify whether orbital shapes and their orientations are derived from experimental observation (exist in atom) or purely theoretical construction
3. comment on a discourse about whether the value of the quantum magnetic number ( $m = -1, 0, +1$ ) corresponds to the orbital orientation  $p_x, p_y, p_z$ , respectively
4. comment on a discourse about whether each type of  $p$  orbital can have any values of the three magnetic quantum numbers ( $m = -1, 0, +1$ )
5. comment on a discourse about whether the quantum magnetic number ( $m = -2, -1, 0, +1, +2$ ) corresponds to the orbital orientation  $d_{x^2-y^2}, d_z^2, d_{xy}, d_{xz}, d_{yz}$ , respectively

**Table 1. Distribution of students' level of understanding for each question in pre-test.**

Question No.	Level of Understanding	Control class (%)	Exp. class (%)
1	<b>True Understanding</b>	<b>4.65</b>	<b>2.22</b>
	• An orbital is the square of the wave function, which represents the high probability area of finding an electron	4.65	2.22
	<b>Partial Understanding</b>	<b>11.63</b>	<b>11.11</b>
	• An orbital is the wave function and space for an electron	11.63	11.11
	<b>Misconception</b>	<b>74.42</b>	<b>74.33</b>
	• An orbital is space with a circular or spherical shape	13.95	9.88
	• An orbital is a trajectory for an electron to rotate around the atomic nucleus	41.86	42.22
	• An orbital is the energy level of an atom with various values	6.98	6.67
	• An orbital is a box that can be filled by an electron	11.63	15.56
	<b>Not Answered</b>	<b>9.30</b>	<b>13.33</b>
2	<b>True Understanding</b>	<b>0</b>	<b>0</b>
	<b>Partial Understanding</b>	<b>9.30</b>	<b>0</b>
	• Atoms are not visible to the naked eye, so orbital shapes and orientations should not exist in atoms. It is a theoretical construction	9.30	0
	<b>Misconception</b>	<b>44.18</b>	<b>24.44</b>
	• Electrons move in 'circular orbitals'; if electrons exist in atoms, then so do orbital shapes and orientations. So, it is an experimental observation	23.25	13.33
	• The existence of the atoms and electrons are observed by experimental observation such as: Thompson experiment, Einstein's photoelectric experiment, etc. Because orbitals are the locations of electrons in an atom, orbital shapes and orientations are also experimental object	20.93	11.11
	<b>Not Answered</b>	<b>46.51</b>	<b>75.56</b>





3	True Understanding	0	0
	Partial Understanding	0	0
	Misconception	86.05	86.67
	<ul style="list-style-type: none"> <li>Generally, the order of the Cartesian axes is x, y, z. Therefore, the numbers are arranged from small to large (<math>m = -1, 0, +1</math>), so the orbitals are as follows: <math>p_x (m=-1)</math>, <math>p_y (m=0)</math>, <math>p_z (m=+1)</math></li> <li>Magnetic quantum numbers can be freely exchanged for each type of p orbital</li> </ul>	74.42	71.11
	Not Answered	11.63	15.56
4	True Understanding	13.95	13.33
	Partial Understanding	0	0
	Misconception	25.58	22.22
	<ul style="list-style-type: none"> <li>Magnetic quantum numbers cannot be freely exchanged for p orbitals because it is an international agreement</li> <li>Magnetic quantum numbers can be freely exchanged for p orbitals. Because <math>p_x</math>, <math>p_y</math>, <math>p_z</math> orbitals have an identical shape, it is not a problem to exchange <math>m = -1, 0, +1</math> for each orbital</li> <li>There is no specific rule to set m for a p orbital. It is only an agreement of chemists</li> </ul>	62.79	62.22
	Not Answered	41.86	42.22
5	True Understanding	20.93	20.00
	Partial Understanding	11.63	15.56
	Misconception	0	0
	<ul style="list-style-type: none"> <li>There is no definite rule to set m for a d orbital. It is only international agreement of chemist. Then, it can be freely exchanged, <math>m = -2, -1, 0, +1</math> or <math>+2</math>, for each d orbital.</li> </ul>	9.30	11.11
	Not Answered	9.30	11.11
		90.70	88.89

After implementation of a learning exercise using Winplot, the effectivity of this computer-aided learning was characterized by the percentage of students in control and experimental class who still have misconception for each post-test question.

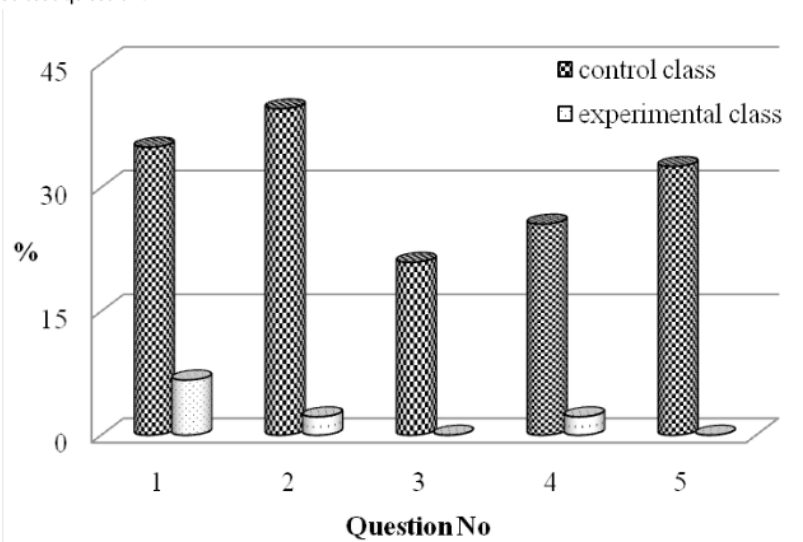


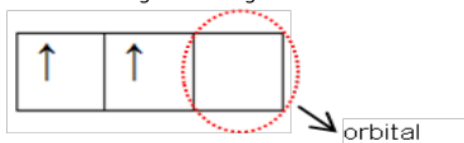
Figure 1: Percentage of students at misconception in post-test for each question.



## Discussion

### *Students' Misconceptions about Orbitals and Quantum Numbers*

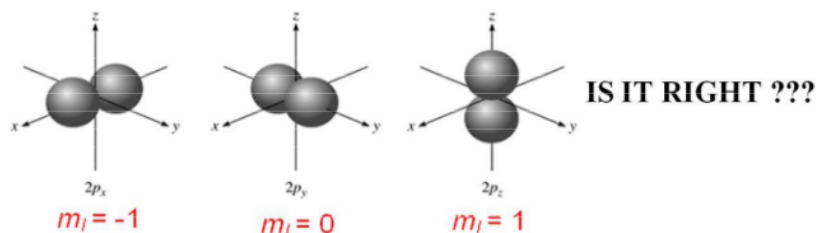
This research was carried out via three main activities: analyzing students' pre-existing concepts, implementing a learning exercise activity using Winplot, and identifying conceptual changes. In analyzing of pre-existing concepts, students were given five questions related to some issues in orbitals and quantum number topic. The first question in this research sought to describe the meaning of an orbital. As shown in table 1, it can be seen that 74.33% of students had a misconception about this question. The dominant incorrect answer was that an orbital is a circular orbit where an electron travels around an atomic nucleus. This answer indicates that students are more confident in using a solar system-like model (Bohr's model) when explaining atomic structure. Apparently, these students believed that Bohr's model is the most advanced atomic structure theory. The atom, in their mind, is arranged by layers or 'shells' that are perceived as an orbital or place of a moving electron. As revealed by in-depth interviews, this misconception arises because learning atomic structure theory in secondary school was restricted to Bohr's theory; subsequently; they directly jumped to the topic of electron configuration. Students thus assumed that Bohr's model is the correct representation of atomic structure and that electron configuration is a different case that has no contribution to atomic structure. The other main misconception is that an orbital is a round or spherical space, represents the energy levels of an atom, or is a 'box' for filling electrons. The last opinion is quite interesting. Students reported that an orbital is a box that can be filled by electrons. As explored in the in-depth interviews, students revealed that this misconception was caused by the habit of their chemistry teacher of presenting the electron filling process in atomic orbitals using a 'box' diagram as demonstrated by figure 2 below:



**Figure 2:** Orbital presented by 'box' diagram.

These responses reveal that the students did not understand the meaning of an orbital in an atom. The second analysis surrounds the question about whether information about orbital shapes and their orientations, as commonly understood from the textbook, is derived from experimental observation or theoretical construction. Some students in control class (9.30%) answered this question correctly, though their rationale was not accurate. They said that atoms are not visible to the naked eye, so orbitals should not exist in atoms. Furthermore, approximately 44.18% students had a misconception of assuming that orbitals can be seen in atoms in the form of balls, twisted balloons, double twisted balloons, etc. They also assumed that if electrons move in 'circular orbits' around atoms, so do orbitals. Another misconception is atoms and electrons were observed experimentally; therefore, if an orbital surrounds an electron, an orbital must be an experimental object. According to this answer, the students did not understand how an orbital is constructed. Students stated that their chemistry teacher had never taught and explained the wave function and its relationship to orbitals.

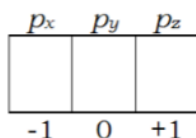
The next question asked students to comment on a discourse about whether  $m = -1, 0, +1$  represents the  $p_x, p_y, p_z$  orientation, respectively, as shown in figure 3.



**Figure 3:**  $m$ -values versus  $p$  orbital orientation relationship that the students were asked about in the second question.



Results of the analysis demonstrated that most students also have a misconception about this topic as also supported by in-depth interviews. They argued that  $p_x, p_y, p_z$  should correspond to increasing magnetic quantum numbers  $-1, 0, +1$ , respectively. The reason is the alphabetic order of Cartesian axes is  $x, y, z$  and the numbers are arranged from small to large number  $(-1, 0, +1)$ , then the orbitals should be  $p_x (m=-1), p_y (m=0), p_z (m=+1)$ . As explored in in-depth-interview, they revealed that their high school chemistry teacher always represented  $p$  orbitals and their corresponding  $m$ -values using the diagram shown in figure 4.



**Figure 4:**  $p$  orbitals and their corresponding  $m$ -values as represented by a high school chemistry teacher.

In addition, another misconception is that  $m$ -values ( $m = -1, 0, +1$ ) did not correspond to specific orientations of  $p$  orbitals. Students argued that each type of  $p$  orbitals can have any values of those magnetic quantum numbers. This error was re-confirmed by the fourth question that asked students to explain whether each type of  $p$  orbital can have any values of the three magnetic quantum numbers ( $m = -1, 0, +1$ ). As predicted by the author, most students answered it can do. They argue that the  $p_x, p_y, p_z$  orbitals have identical shapes, so each  $p$  orbital can have all three quantum numbers. Another misconception is that there is no specific rule to set  $m$  for a  $p$  orbital. Students expected that the  $m$ -values for each type of  $p$  orbitals is an International agreement of chemist. This indicated that students are really confused by the relationship of  $m$  and orbital shapes or orientations.

The last question is in line with the fourth question but refers instead to the  $d$  orbital. Interestingly, approximately 88.89% of students in experimental class and 90.70% of students in control class did not answer the question regarding the relationship of  $m$ -values with  $d$  orbital orientation. This information indicated that students in general did not understand  $d$  orbital compared to  $p$  orbitals. These students stated that their teacher never showed the relationship of  $m$ -values for the  $d$  orbital. Moreover, approximately 9.30% of students in control class and 11.11% of students in experimental class showed misconception by answers that  $m$ -values have no specific rules and each type of  $d$  orbital can have any values of the magnetic quantum numbers. They more likely believed that  $m$ -values are only an international agreement, have no definite rule, and are not specific for each type of orbital. By these pre-existing concept analysis, it is apparent that most students did not have a comprehensive understanding of orbitals and quantum numbers. This motivates us to use simple and real-time visualization tool named Winplot in a learning exercise activity as an alternative strategy to counter misconceptions related to these questions.

#### *Learning Exercise Using Winplot*

This research is intended to counter student misconceptions about 6 topics that have been explained to them before. In this computer-based strategy, students were given a worksheet that contained two assignments. First, they were asked to draw an atomic orbital manually and list the corresponding  $l$  and  $m$  quantum numbers based on their pre-existing concepts. The second task contained a Winplot code that represents the mathematical equation for each  $l$  and  $m$  quantum number. They were asked to input the code into Winplot, draw the result obtained and list the corresponding  $l$  and  $m$  quantum numbers. Furthermore, students were asked to compare their first and second answers, evaluate the similarities and differences, self-correct their first answer, and explain their new findings. In the worksheet, students were also asked some explorative questions about the meaning of orbitals, how they are obtained and their relationship to quantum numbers.

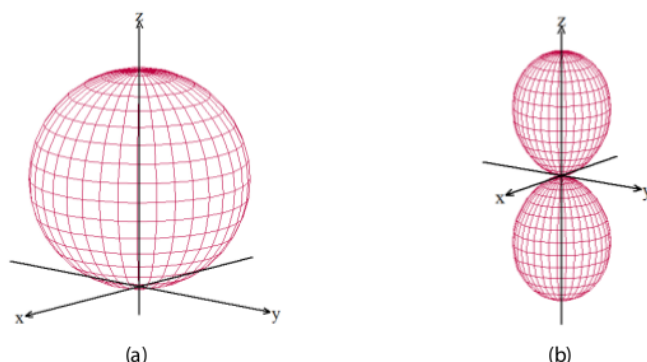
#### *Conceptual Changes*

A post-test was conducted to examine students' conceptual changes after implementing learning exercise using Winplot. The effectivity of this strategy was indicated by potency to decrease number of students who had misconception. The results demonstrated dramatic conceptual changes in post-test after the learning exercise activity using Winplot, as presented by figure 4. According to Figure 4, approximately 34.88% of students in control class





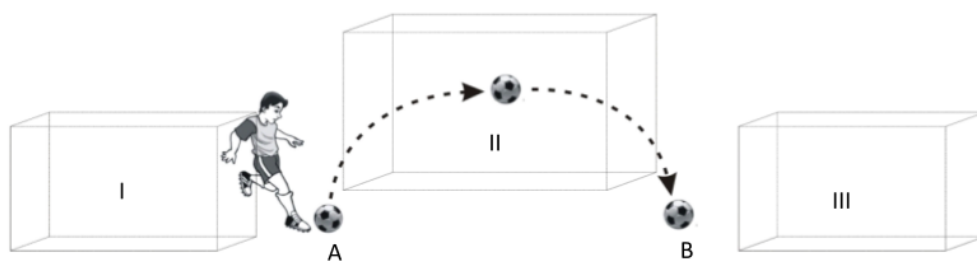
still had a misconception of the first question, whereas experimental class showed only 6.67%. After implementing a learning exercise using Winplot, most of students understand that an orbital is the square of the mathematical wave-function that gives information about the maximum probability of finding an electron in an atom. Learning exercise activity for the first question asked students to compare visualization between wave function and square wave function for  $p_x$ ,  $p_y$ ,  $p_z$ . By doing this activity, students will understand that visualizing wave function will never generate best representation of  $p$  orbitals, except visualizing of its square as shown in figure 5.



**Figure 5: Comparison of Visualization Result of (a) Wave function and (b) Square Wave Function of  $p_z$  Orbital Generated by Winplot.**

Furthermore, 11.11% of students in experimental class displayed a partial understanding, as they noted that an orbital is the square of the wave-function without considering the physical interpretation. However, this partial understanding is not actually fatal, as those students would be given additional tutorial and mentoring to get complete conceptual understanding of orbitals. Significant conceptual changes also occurred in the second question. After students found that square wave function produces orbital representation, almost all of the students in experimental class changed their conception from an experimental to theoretical mindset, only one student (2.22%) still hold his wrong concept. Compared to experimental class, 39.53% of students in control class still had misconception. This indicated that constructing orbitals in students' own project makes them believe that all orbitals' information is coming from mathematics. In their exercise activity for the second question, students were given questions consecutively with simple analogy such as:

Question 1: "a stationary ball ( $t = 0$ s) was kicked from A point to B point as shown in figure 6, where it will be required 5 seconds to arrive in B. Where is the higher probability area in finding a ball at  $t = 2$  second; box I, box II, or box III?"



**Figure 6: An analogy of the existence of orbital.**



Answer 1: "box II"

Question 2: "in your opinion, does this "box" really exist in real life?"

Answer 2: "no way, box is only a representation of the higher probability area in finding a moving ball for  $t = 0.5$  second"

Question 3: "can the box be modelled using a mathematical equation?"

Answer 3: "yes, it is"

Students were informed that the "box" is analog with orbital and "ball" is electron. Box is only the representation of the highest probability area in finding a ball, which does not actually exist in real life. Analog with the box, orbital is the highest probability area in finding electrons in an atom. By visualizing orbital from its wave functions and enriched further by simple analogy, students in experimental class realized that orbital shapes and its orientations (spherical symmetric, twisted balloon, double twisted balloon, etc.), as commonly understood from a textbook are only mathematical constructions, do not really exist in the atom. As noted in in-depth interview, students were never taught how to construct orbitals by themselves and where orbitals come from in secondary school. Their secondary chemistry teachers only said that atoms are composed of protons and electrons in which electron stays in a space named orbital. By this argument, students assume that orbitals really exist in atoms and this leads to misconception.

Questions number 3-5 asked students for the link between orbitals and quantum numbers. Surprisingly, all of the students in experimental class had true understanding after implementing exercise using Winplot visualization tool. This indicated that Winplot has high capability in real-time presenting the link between orbitals and quantum numbers. In contrary, students in control class still had many students at misconceptions. There are 20.93%, 25.58%, and 32.56% for question number 3, 4, and 5. In learning exercise activity, students were given angular function of  $p$  orbital with its related quantum numbers as explained in standard physical chemistry textbook that generally used in our class as shown in table 2. Then, students convert the equations to Winplot code and plotting it in the classroom. After those treatments, all students agreed that  $m$ -values cannot be freely exchanged for each type of  $p$  orbital. They also agreed that  $m=0$  is only for  $p_z$  and  $m=\pm 1$  for both  $[p_x, p_y]$  because of the mathematical consequences.

**Table 2. Wave function and its related quantum numbers for  $p$  orbitals (McQuarrie, 1983).**

$l$	$m$	Orbitals	Angular Function $(Y_l^m)(Y_l^m)$
0	0	s	$Y_0^0 = \frac{1}{\sqrt{4\pi}}$
1	0	$p_z$	$Y_1^0 = \frac{\sqrt{6} \cos \theta}{2\sqrt{2\pi}}$
	$\pm 1$	$p_x$	$\frac{1}{\sqrt{2}}(Y_1^1 + Y_1^{-1}) = \frac{\sqrt{3} \sin \theta \cos \theta}{2\sqrt{\pi}}$
	$\pm 1$	$p_y$	$\frac{1}{\sqrt{2}i}(Y_1^1 - Y_1^{-1}) = \frac{\sqrt{3} \sin \theta \sin \theta}{2\sqrt{\pi}}$



$l$	$m$	Orbitals	Angular Function $(Y_l^m)(Y_l^m)$
2	0	$dz^2$	$Y_2^0 = \frac{\sqrt{10}(3 \cos^2 \theta - 1)}{4\sqrt{2\pi}}$
	$\pm 1$	$dxz$	$\frac{1}{\sqrt{2}}(Y_2^1 + Y_2^{-1}) = \frac{\sqrt{15} \sin \theta \cos \theta \cos \Phi}{2\sqrt{\pi}}$
	$\pm 1$	$dyz$	$\frac{1}{\sqrt{2}i}(Y_2^1 - Y_2^{-1}) = \frac{\sqrt{15} \sin \theta \cos \theta \sin \Phi}{2\sqrt{\pi}}$
	$\pm 2$	$d_{x^2-y^2}$	$\frac{1}{\sqrt{2}}(Y_2^2 + Y_2^{-2}) = \frac{\sqrt{15} \sin^2 \theta \cos 2\Phi}{4\sqrt{\pi}}$
	$\pm 2$	$dxy$	$\frac{1}{\sqrt{2}i}(Y_2^2 - Y_2^{-2}) = \frac{\sqrt{15} \sin^2 \theta \sin 2\Phi}{4\sqrt{\pi}}$

In contrary, almost all students in control class could not understand the relationships of orbitals and quantum numbers. Number of students who had misconceptions on pre-test are not significantly different in post-test. This indicated that conventional strategy without the help of computer visualization cannot give a significant change to construct this concept. Otherwise, after applying learning exercise using Winplot, in line with that, in the case of the  $d$  orbital in question 6, students also understood that  $m=0$  is only for  $d_z^2$ ,  $m=\pm 1$  for both  $[d_{xz}, d_{yz}]$ , and  $m=\pm 2$  for both  $[d_{x^2-y^2}, d_{xy}]$  after implementation of learning exercise activity. This strategy is really effective to construct true conception about orbitals and quantum numbers because it provides students to real-time plotting orbitals from its origin equation.

Finally, this research determined that applying Winplot in a learning exercise activity is an effective computer-based strategy in countering misconceptions related to orbitals and quantum numbers. By transforming equations into 3D visualizations, students obtained important information, such as (a) the shape and orientation of atomic orbitals that are commonly known from a chemistry textbook are derived from mathematical construction as opposed to experimental observation, (b) the relationship between magnetic quantum number and orbital orientation, and (c) the  $m$ -value is specific and cannot be freely exchanged for each type of orbital. Due to its advantages, Winplot is highly recommended for wide use in learning chemistry at schools or universities.

## Conclusions

These findings informed some misconceptions related to orbitals and quantum number topic held by first-year undergraduate chemistry students and a novel strategy to counter those misconceptions. As described in students' responses to pre-test questions, students were confused about how orbitals are constructed and the relationship between orbitals and  $m$ -values. After a learning exercise activity applied, most of the students showed significant conceptual changes. This research demonstrated that students' learning exercise using Winplot is an effective computer-based learning strategy to counter several student misconceptions about orbitals and quantum numbers.

## Acknowledgements

Authors declare many thanks to Anonymous Reviewers, who give constructive suggestions to the content of this manuscript. Big thanks is also addressed to Mr. Fajar Arrasyid, A Graduate Student of Chemical Education, Faculty of Teacher Training and Education, University of Lampung, for his contribution in providing high quality pictures in the manuscript.





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Received: June 22, 2016

Accepted: July 30, 2016

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# A Learning Exercise using Simple and RealTime Visualization TOOL to Counter Misconceptions about Orbitals and Quantum Numbers

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