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Learning Quantum Chemistry via Visual-conceptual Approach: Students' Bidirectional Textual and Visual Understanding

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Abstract

Most undergraduate chemistry courses and a few high school honors courses, which focus on physical chemistry and quantum mechanics, are highly mathematically-oriented. At the Technion, Israel Institute of Technology, we developed a new module for high school students, titled *Chemistry – From “the Hole” to “the Whole”: From the Nanoscale to Microelectronics*. The module is based on a qualitative approach to teaching quantum chemistry, emphasizing interdisciplinary real-life applications and integration of visualization. While aimed at honors high school chemistry students, the module was also partially implemented and assessed in an undergraduate chemistry course. The research objective was to investigate the effect of the module on the visual and textual understanding of quantum mechanical concepts among 122 honors and 65 volunteer undergraduate chemistry students. The research tools included students' pre- and post-questionnaires. High school honors and undergraduate students, who were exposed to the module, improved significantly their textual and visual understanding of quantum mechanical concepts and their ability to move across illustrations and explanations. Honors and undergraduate students minimized the gap that had existed between them in terms of integrating micro and quantum levels into their post-questionnaire answers. Our findings augment the current set of the four chemistry understanding levels – macro, micro, symbol and process – by adding the quantum mechanical level as a fifth level of chemistry understanding. The study contributes to teaching physical chemistry by providing a tool for learning, assessment, and research of chemistry understanding via both visual and textual modes.

Key words: quantum mechanics, physical chemistry, textual and visual understanding, chemistry understanding levels, visual-conceptual approach, quantum mechanical level

Introduction

The conventional approach to teaching undergraduate physical chemistry and quantum mechanics courses is mathematically-oriented, and often lacks emphasis on qualitative understanding of underlying principles. We introduce a visual-conceptual approach to teaching quantum mechanical principles to honors high school students, which can also benefit undergraduate students. Our approach integrates visual representations with textual explanations that focus on understanding chemical principles and concepts. Research over the past decade has indicated the existence of difficulties in teaching and learning topics related to quantum mechanics in both physics and chemistry courses (Ireson, 2000; Taber, 2005; Papaphotis and Tsaparlis, 2008). These difficulties stem from the fact that quantum mechanics involves abstract concepts and complex theories. Integration of visual representations might alleviate these

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3 difficulties by promoting better understanding and meaningful learning of science. In line with
4 this approach, we have developed, implemented, and assessed a new learning module that
5 focuses on quantum chemistry, titled *Chemistry – From “the Hole” to “the Whole”: From the*
6 *Nanoscale to Microelectronics*¹ (Sasson et al. 2007). The module includes abstract topics that
7 rely on quantum mechanics theories with an emphasis on a qualitative approach and integration
8 of visualizations. The research described here explores the effect of learning quantum chemistry
9 through this qualitative approach and the integration of visualizations on developing textual and
10 visual chemical understanding among chemistry high school honors and undergraduate students.
11 As we were studying the students’ responses, we realized that a fifth chemistry understanding
12 level—the quantum level—can and should be added to the current four levels. We elaborate on
13 this in the discussion section.
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17 **Theoretical background**

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20 Research on difficulties in teaching and learning quantum mechanical concepts calls for
21 strategies that promote students' conceptual understanding and minimize their misconceptions
22 regarding the atomic structure. Our learning module integrates visualization and the current four
23 chemical understanding levels—macroscopic, microscopic, symbol, and process—into learning
24 quantum chemistry; thus, we review the literature concerning the teaching and learning of
25 quantum mechanical concepts as well as literature that emphasizes visualizations and the four
26 chemistry understanding levels as key aspects for teaching and learning chemistry for conceptual
27 understanding.
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30 **Teaching and learning quantum mechanical concepts**

31 Researchers point out difficulties and obstacles in teaching and learning quantum mechanical
32 concepts at the high school and university levels (Harrison and Treagust, 1996; Stefani and
33 Tsaparlis, 2009). Findings indicate that high school students, college students studying for
34 university entrance level exams, and students at the undergraduate level experience difficulties
35 rethinking their previous knowledge while creating alternative conceptions of the atom model,
36 orbitals, energy levels, and related ideas (Harrison and Treagust, 1996; Petri and Niedderer,
37 1998; Taber, 2005; Papaphotis and Tsaparlis, 2008).

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39 One of the most prevalent reported obstacles is the difficulty in understanding abstract concepts.
40 Students in middle and high school tend to depict atoms and molecules as discrete and concrete
41 structures and thus prefer illustrations of the orbit model and planetary (also referred to as ‘solar
42 system’) model of the atom (Harrison and Treagust, 1996; Cokelez, 2012). They usually use the
43 word ‘orbital’ as a synonym for an ‘orbit’ and think that electrons rotate around the nucleus like
44 the planets rotate around the sun (Tsaparlis and Papaphotis, 2002). Tsaparlis (1997) raised the
45 question whether quantum mechanical concepts should be taught at the secondary school and
46 cited Gillespie (1991, 1996) that recommended emphasizing electron density and VSEPR rather
47 than concepts such as orbitals. These recommendations were for teaching both secondary school
48 students and even introductory courses for students at the college and university level. Taber
49 (2005) argued that even when college students, who are studying for university entrance level
50 exams, embrace the term orbital, some still tend to use it to re-label their existing conceptions of
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55 ¹ In what follows, we refer to the module as *Chemistry – From the Nanoscale to*
56 *Microelectronics*
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3 electron 'path' as it 'circles' the nucleus. Cokelez (2012) showed that some students in junior
4 and high school illustrate what he called 'composition models', which are more complex and
5 abstract. Yet he claimed that students' knowledge of and experience with the atomic model is not
6 sufficient, and that the atomic model theory should be part of the curriculum in all the science
7 domains.
8

9 Tsaparlis and Papaphotis (2002) argued that high school students fail to understand the
10 probabilistic nature of atomic orbitals and retain a deterministic perspective. Students do not
11 fully understand atomic and molecular orbitals. They are confused between the various atomic
12 and orbital representations and misinterpret them. Furthermore, undergraduate students have
13 difficulties identifying the mathematical characteristics of quantum mechanical concepts and the
14 different forms of mathematical equations related to these concepts (Tsaparlis, 1997; Stefani and
15 Tsaparlis, 2009).
16

17 One of the problems that lead to students' misconceptions about the atomic model and the
18 quantum mechanical concepts is that students at both high school and undergraduate levels tend
19 to develop hybrid models (Justi and Gilbert, 1999; Stefany and Tsaparlis, 2009; Taber, 2001a).
20 Students merge and use in parallel different models, such as aspects of historical models and
21 aspects of the current acceptable model of the atom. They create a mental model that integrates
22 different models which they treat as coherent (Petri and Niedderer, 1998; Justi and Gilbert, 1999;
23 Justi and Gilbert, 2000, Papaphotis and Tsaparlis 2008).
24

25 Learning the atomic model by depicting the planetary model or Bohr model might be useful for
26 middle and high school students, helping them in integrating the idea of shells. However, a
27 learning progression approach should be taken, where a scheme of four stages of conceptual
28 understanding of the atomic structure and electrical forces are introduced. The highest stage of
29 understanding includes quantum mechanics models. Only few students described atomic models
30 and electrons in terms of probability and electron density, while others kept using language that
31 is generally associated with classical mechanics to describe electron motion (Stevens et al.
32 2010).
33

34 Understanding the concepts of 'probability of finding electrons' and 'energy quantization' are
35 necessary as a basis for comprehension of the quantum mechanics model of the atomic structure
36 when learning at the undergraduate level (Park and Light 2009). However, high school chemistry
37 textbooks usually do not provide learners any reason to accept the quantum mechanics model
38 instead of the Bohr model (Shiland, 1997).
39

40 Looking at examples from the literature of teaching quantum chemistry, there are different
41 strategies that were found beneficial to some extent. These include a qualitative teaching
42 approach (Kalkanis et al., 2003), use of simulations and animations for teaching nanotechnology
43 based on quantum theory (Xie and Lee, 2012), and learning with devices whose mechanism can
44 only be explained by conceptually understanding quantum chemistry (Green et al., 2009;
45 Zollman et al., 2002).
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47 Our unique approach integrates extensive use of a variety of visualizations with everyday
48 applications and a visual-conceptual teaching approach. Furthermore, it cater to both high school
49 and undergraduate students. Concepts are taught over a relatively long period of time with
50 multiple experiences with quantum chemistry concepts. This potentially leads to deep conceptual
51 understanding of atomic and molecular structures.
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53 **Visualization in learning sciences and chemistry**

54 Visual representations, such as graphs, diagrams, visual models, and inscriptions, play a key role
55 in teaching and learning sciences (Barak and Dori, 2005; Dori and Belcher, 2005; Kozma and
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Russell, 2005a). 'Representational competence' is part of meaningful understanding of chemistry concepts and includes the ability to use a variety of representations or visualizations, including communicating, selecting appropriate representations, using them for explaining chemical phenomena, and integrating new knowledge with existing knowledge (Roth et al., 1999; Kozma and Russell 2005a). Bowen and Roth (2005) claimed that representations that use mathematical equations are highly abstract, and that students find them to be the most difficult feature of science learning (Roth and Bowen, 1994).

There are several key principles, suggested by Wu and Shah (2004) that can assist students with understanding chemistry concepts and to develop representational skills and visuospatial thinking. These include (1) exposing students to the same information in a multitude of formats and descriptions, (2) making linked referential connections between representations visible in order to enable students to construct conceptual connections from these multiple representations, (3) presenting the dynamic and interactive nature of chemistry, and (4) encouraging the transformation between 2D and 3D. Mayer (2002) described learning processes in which students use words and pictures based on three assumptions (a) people use the visual-pictorial channel and the auditory-verbal channel, (b) these channels can become overloaded when too many words and pictures are involved in the learning, and (c) meaningful learning occurs when students are actively engaged and process their learning via practicing the two channels.

Researchers also found that computer-based visualization tools and computerized molecular modeling may help students improve their ability to make transformations between 2D and 3D models. In turn, this ability may help students develop understanding of chemical principles (Kaberman and Dori, 2009; Wu et al., 2001). When it comes to quantum theoretical concepts, visualization enables the construction of a richer set of concepts (Gunel et al, 2006). It can also be used to identify students' mental models of the particulate nature of matter (Ben Zvi et al., 1987; Margel et al., 2004; Nyachwayaa, et al., 2011) and of atoms and molecules while investigating students' illustrations. Specifically, visualization can enhance students' understanding of shape and size of the atom and the probabilistic nature of the atom orbitals (Cokelez, 2012; Papaphotis and Tsaparlis 2008; Park and Light, 2009).

Chemistry understanding levels

Students' chemical understanding can be evaluated by their comprehension of and transfer between the four levels, which include the macro, micro, symbol, and process levels (Dori and Hameiri, 2003; Kaberman and Dori, 2009). Initially, researchers had argued that chemistry is taught and understood at three levels: the microscopic, also referred to as sub-microscopic – the particulate nature of matter level; the macroscopic – the sensory level; and the symbolic, which is also referred to as the representation level (Johnstone, 1991; Gable, 1993, 1998). Dori and Hameiri (2003) have added the fourth, process level of chemistry understanding, which accounts for the dynamic nature of chemical reactions and the relationship between the macroscopic, microscopic and symbolic levels. Jensen (1998) proposed a model, which he described as "the vision of the overall logical structure of Chemistry" (p. 679). This model refers to chemists and teachers as they view the logical organization of chemistry, although it can be translate by teachers into their teaching, it does not refer specifically for students. This is unlike the four chemistry understanding levels, which can be used by students as a metacognitive tool for monitoring their understanding of chemistry concepts and processes (Kaberman and Dori, 2009). Jensen's model included three levels: molar, molecular and electricity. The molar level in Jensen's model had similar meaning as the macroscopic level, and the molecular level is what we refer to as the microscopic level. Jensen did not mentioned the process level (which was added

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3 by Dori and Hameiri (2003) but we can see some resemblance between the process level and the
4 time dimension mentioned in Jensen's article, since they both have dynamic aspect we discuss
5 when we refer to the process understanding level.

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7 Researchers have claimed that understanding microscopic and symbolic representations is
8 especially difficult for students because these representations are invisible and abstract, while
9 students' thinking relies mainly on sensory information (Ben-Zvi et al., 1987; Gable, 1993; Wu et
10 al., 2001). Still, meaningful learning may be enhanced through visualizations, including physical
11 models, computerized visualizations, animations, and drawings. Visualizations contribute to
12 improving students' ability to use the chemistry understanding levels and move across them
13 (Barnea and Dori, 1999; Dori et al., 2003; Kozma and Russell, 2005b).

14
15 Chemistry understanding levels serve also as a metacognitive tool for students when they explain
16 chemistry phenomena (Herscovitz et al., 2012). In his review, Taber (2001b) described the
17 difficulty students face when they need to traverse the different levels and the importance of
18 using the macro, representation, and sub-micro levels. When discussing quantum chemistry,
19 Taber (2001b) cited a PhD dissertation (Van Hoeve-Brouwer, 1996) that had suggested adding
20 the quantum level.

21
22 In this study, we propose adding a fifth, quantum chemistry understanding level on top of the
23 four we have been using in previous studies (Dori and Hameiri, 1998, 2003; Dori and Sasson,
24 2008; Kaberman and Dori, 2009) and use it for both teaching and assessment.

25 26 27 **Research objectives**

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29 Considering the difficulties students encounter while learning quantum chemistry and the
30 potential of visualization combined with understanding chemistry at different levels to improve
31 conceptual understanding, we focused on the following research objectives:

- 32 1. Investigating the effect of the visual-conceptual approach in the new module on high school
33 honors chemistry and undergraduate students' understanding of quantum mechanical
34 concepts, and
- 35 2. Comparing the learning outcomes of three research sub-groups in terms of visual and textual
36 understanding of chemistry in general and of quantum mechanics in particular.

37 38 39 **Context**

40
41 The new module for honors high school students, *Chemistry – From the Nanoscale to*
42 *Microelectronics*, developed at the Technion, includes abstract topics from quantum mechanics
43 theory. It focuses on chemical properties derived from the electronic structure of substances:
44 orbitals in atoms and molecules, and energy bands in bulk semiconductors. The latter topic had
45 never been taught in honors chemistry courses in Israel; therefore, no comparison group could
46 have been established.

47
48 There are few research articles on teaching semiconductors to high school students. The majority
49 of research articles have appeared in engineering and physics publications, which focus on
50 quantitative, mathematical, and device aspects, rather than chemical aspects (Santos et al., 2009;
51 Yeow and Ling, 1999). When the chemical aspects of a semiconductor are described, the
52 explanations are based on the classic model and apply concepts such as covalent bonds,
53 additional electrons, and “holes” rather than the quantum model (García-Carmonaa and Criado,
54 2009; Ren et al., 2008). Teaching semiconductors as an application of the electronic structure of
55 solids using quantum theory has received almost no attention in the literature.

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3 While conventional approaches to teaching undergraduate physical chemistry and quantum
4 mechanics courses are mathematically-oriented, we have adopted a visual-conceptual approach
5 to teaching quantum chemistry. This approach is of a qualitative nature; it emphasizes
6 interdisciplinary real-life applications and integrates ample visualizations. For example, while
7 learning the topic of the electronic structure of molecules and its key concepts, such as molecular
8 orbitals, bonding, anti-bonding, HOMO (Highest Occupied Molecular Orbital), and LUMO
9 (Lowest Unoccupied Molecular Orbital), students investigate questions like “why do organic
10 pigments have colors?”, and the phenomenon of stick lights is explained. The characteristics of
11 the module include numerous visualizations and animations, which are exemplified in Appendix
12 1.

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15 Since most high school students lack proper background in mathematics at the required level, our
16 qualitative approach helps bypass the introduction of mathematical aspects of quantum theory.
17 While aimed at honors high school students, as noted, this module was also assessed and used
18 during an undergraduate mathematical-oriented quantum chemistry course.
19

20 **Research participants**

21 The research participants were (1) 12th grade chemistry honors students from eight high schools
22 in Israel over two academic school years (N=122), who studied the module in its entirety and (2)
23 undergraduate students (N=65) who volunteered to participate in the research and studied the
24 module in one academic year as part of a quantum chemistry course titled *Introduction to*
25 *Quantum Mechanics and its Applications in Chemistry*.

26
27 The undergraduate students were majors in three domains: chemistry, biochemistry, and
28 electrical engineering. The honors students were divided into two sub-groups: intermediate- and
29 high-academic level. The undergraduate students were also divided into two sub-groups: sub-
30 group 1, "Visual-Conceptual-oriented" (ViCo-oriented) – students who participated in a short-
31 term enrichment course that included the topics of the module, focusing on a visualization and
32 qualitative approach, and sub-group 2, "Mathematical-oriented"(Math-oriented) – students who
33 participated in a short-term mathematical-oriented enrichment course, which included topics
34 taught in the quantum mechanics course.
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37 The undergraduate students took the enrichment course in addition to the regular academic
38 course. The course comprised of six sessions taught over three weeks. The students chose to
39 participate in sub-group 1 or sub-group 2 based on their academic schedules, without being
40 provided with any specific information about the content of the enrichment given to each sub-
41 group.
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43 **Research tools**

44 The research tools included pre- and post-questionnaires aimed at assessing thinking skills and
45 chemistry understanding. The high school students responded to the pre-questionnaires prior to
46 the onset of the module, and the post-questionnaire was administered to the students at the
47 completion of the module. The undergraduate students responded to the pre-questionnaire during
48 the first week of the semester and to the post-questionnaire during the semester after they had
49 finished the enrichment course.
50

51 The pre- and post-questionnaires, which included open-ended questions, were administered for
52 the purpose of assessing two thinking skills: (a) the ability to apply visual and textual modes to
53 explain chemical phenomena in terms of quantum mechanical concepts, and (b) the
54 understanding of various representation and visualization modes, including molecular drawings,
55 graphs, diagrams, and illustrations.
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3 The pre-questionnaire was based on topics from chemical structure and bonding, while the post-
4 questionnaire focused on quantum mechanical content. In order to assess students' knowledge
5 and the above two thinking skills, students were requested to perform the following three
6 assignments.
7

- 8 A. Choose one of the concepts from the list below and describe it using a drawing, a
9 diagram, or a model.
10
11 B. Choose another concept and explain it textually using an example.
12
13 C. Explain a given illustration (see example in Appendix 2, which relates to the ability to
14 explain the concepts of bonding and anti-bonding molecular orbitals).

15 Concepts for assignment A and B included atomic orbital, molecular orbital, energy levels,
16 LOMO orbital, and N type semiconductors.

17 For the purpose of assessing students' ability to describe and explain new concepts using both
18 visual and textual modes, and to understand representations and visualizations, we developed a
19 dedicated assessment tool for each one the three assignments. The tool (see Appendix 3)
20 consisted of a detailed rubric designed to assess both the textual and the visual modes. Each
21 mode was graded independently using qualitative content analysis followed by a quantitative
22 score. Although 'assignment A' was aimed to assess the visual mode and 'assignment B' was
23 aimed to assess the textual mode, students often used both modes in the assignment. In these
24 cases we assessed the two modes used in the same assignment and the extent to which they
25 matched (see Appendix 3).
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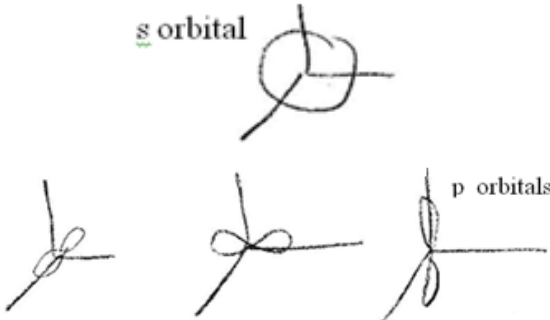
27 Each assignment set was scored separately according to several categories, some of which were
28 identical across the three assignments.
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30 A common criterion to both modes was the correctness of the textual or visual (drawing or
31 illustration) explanation. A non-quantum mechanical illustration, such as depiction of an atom
32 using historical models, the nuclear model (Park and light, 2009), Rutherford (planetary) type
33 model, (Wheeldon, 2012), or a planetary or solar system model (Harrison and Treagust, 1996;
34 Stevens et al., 2010; Taber 2001a) was categorized as a "naïve illustration". Additional
35 categories, specific to the visual mode, were the number of illustrations and the complexity
36 (richness) of each illustration. Richer and more detailed illustrations were assumed to reflect
37 deeper understanding of the concept the students had chosen to explain and better visual
38 capability to draw a meaningful representation of that concept.
39

40 Understanding of chemistry on both the textual and the visual modes was assessed via the four
41 chemistry understanding levels using a method developed in prior research for textual responses
42 (Dori and Sasson, 2008; Kaberman and Dori, 2009). Analyzing the results from students' pre-
43 and post-questionnaires, we added the quantum-mechanical level as a fifth chemistry
44 understanding level. This level includes the ability to describe the electronic structure of atoms,
45 molecules, and solid state materials in terms such as discrete energy levels, atomic and molecular
46 orbitals, energy bands, and absorption and emission spectra, all stemming from the theory of
47 quantum mechanics.
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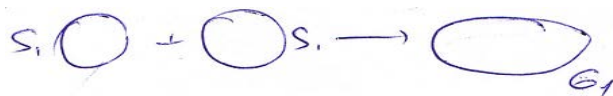
49 Each of the assignments A, B, and C was analyzed separately. In each assignment performed by
50 each student, the number of micro explanations, quantum explanations, or the combination of
51 both were counted. In the findings section, we present the distribution of the number of the micro
52 explanations, quantum explanations, and combined micro and quantum explanations as the sum
53 of explanations students in each of the three groups gave in the three assignments. Table 1
54 presents examples of students' responses for each one of the assignments.
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Table 1 Examples of students' answers and their analysis in assignments A, B, and C.

Assignment	Students' responses	Representation Type	Category	Explanation
A	<p>The concept: atomic orbital</p>  <p><i>In each orbital there are n^2 electrons. Each couple of electrons is occupied in inverted spins (+1/2, -1/2). There are s, p, d, orbitals etc. (Undergraduate student)</i></p>	Visual representation	Number of drawings	Two connected illustrations of s and p orbitals
			Character of drawing	The illustration focused on the quantum level
			Correctness	Correct illustration
			Complexity	More than three items (p and s orbitals, axis, names)
		Textual representation	Correctness	Partially correct. (in one orbital only 2 electrons can be occupied)
		Chemistry understanding levels	quantum level	
		Connection between the modes of representation	Coherence	Correct matching
B	<p>The concept: molecular orbital</p> <p><i>A molecular orbital is an area in which the probability to find an electron with the suitable energy is high. A molecular orbital is formed by the sum or by the subtraction of atomic orbital which also represents the area in which the probability to find the electron is high, but in the atom not in the molecule. For example</i></p>	Textual representation	Correctness	Partially correct: the student confuses the spatial drawing of an orbital with the definition of an orbital (the orbital is defined for the

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the hydrogen molecule:
(Undergraduate student)



Visual
representation

entire space). A
detailed
explanation

Correctness

A correct example

Chemistry
understanding levels

Micro and
quantum levels

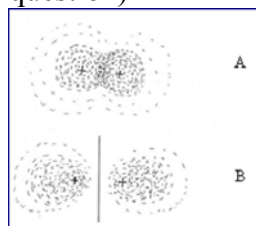
Correctness

Correct illustration

Complexity

More than three
items (s and σ
orbitals, names)

C (See Appendix
3 for the entire
question)



*i. The symbol “+” represents the atomic
nucleuses.*

*ii. The vertical line represents the nodal
plane in which there is zero probability to
find an electron.*

*iii. The dot's density represents the
probability to find electrons in the orbital
space around the nucleus.*

*iv. Orbital B is higher in its energy – it is an
anti-bonding orbital (the electrons are
further from the two nucleuses and have
higher energy from electrons that are
between the space of the two nucleuses)*

(High school student)

Textual
representation

Correctness and
detailed content

Correct
explanation to sub-
questions i – iii and
correct answer to
sub-question iv.

Chemistry
understanding levels

Micro and
quantum levels

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3 The overall score in each assignment was summarized and normalized on a 1-to-100 scale. The
4 average score of the three assignments was statistically analyzed. One-tenth of all the students'
5 responses were scored and validated by four chemistry educational experts, achieving 90% inter-
6 raters reliability.
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8 **Findings**

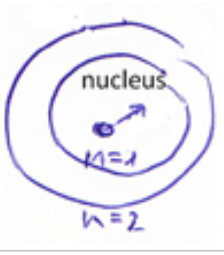
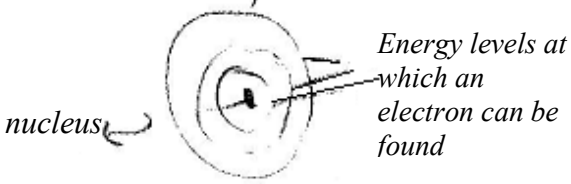
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10 The questionnaires were analyzed, first qualitatively and then quantitatively, using the
11 assessment tool presented above. In this section, we present the qualitative findings followed by
12 the quantitative findings of understanding quantum mechanical concepts and principles regarding
13 the textual and visual chemical understanding.
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15 **Understanding concepts and principles in quantum mechanics – qualitative analysis**

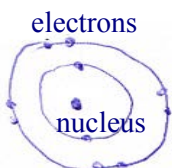
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17 The content analysis of students' responses revealed interesting new combinations in describing
18 the concepts. Students used several levels of understanding, particularly the micro and quantum
19 levels. The students used a variety of models, some of which demonstrated deep understanding
20 of the explained concept, while others mixed previous, non-quantum models, indicating
21 incomplete conceptual understanding (Justi and Gilbert, 1999; Stefany and Tsaparlis, 2009;
22 Taber, 2001a). The qualitative analysis exposed a need to teach three subjects: the electronic
23 structure of the atom, the electronic structure of the molecule, and the solid state.
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25 **Understanding concepts related to the atom's electronic structure.** Students'
26 responses reflected a large variety of thinking skills and understanding levels. As an example, we
27 consider the concept of discrete energy levels, which is essential to the understanding of
28 quantum mechanics, and which the students were asked to illustrate and explain. Students'
29 responses reflected four evolutionary stages of quantum mechanical understanding: (1) the naïve
30 model, such as the planetary (solar system) model of the atom (Harrison and Treagust, 1996;
31 Stevens et al., 2010) or nuclear model (Park and Light, 2009), which do not involve the quantum
32 mechanical probabilistic concept, (2) the hybrid model, which merges the quantum mechanics
33 model with previous models, (3) the visual-conceptual probabilistic quantum mechanics model,
34 which had been taught in the module, and (4) the generic mathematical model of the quantum
35 mechanics theory. Table 2 provides examples of high school and undergraduate student
36 responses to the post-questionnaire assignment of describing the concept of discrete energy
37 levels, showing all the above four stages of quantum mechanical understanding.
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Table 2 Students' responses to the description of the energy levels concept

Students' responses	Analysis
<p><u>Naïve model:</u> <i>Every material has electrons which surround the nucleus. They occupy divided shells. It is easier to take out/ionize the electrons on the outer shell of the atom which means that less energy has to be invested.</i></p>	<p>The students' textual explanation focuses on the micro level rather than on the quantum mechanical concepts that were taught in the module. The illustration presents a correct abstract description of the quantum mechanical energy shells model of the atom, but it is not clear whether the student understands the difference between the naïve model and the probabilistic quantum mechanics model.</p>
<div style="text-align: center;">  </div> <p>(High school student)</p>	
<p><u>Hybrid model:</u> <i>The energy level at which an electron can be found in an atom. Relates to the concept $E_n = \frac{\pi^2 \hbar^2}{2mL^2} n^2$ while n represents energy levels at which a particle can be found</i></p>	<p>The student's response represents a hybrid model, which merges quantum mechanics model and previous model. The text relates to the quantum model of discrete energy levels, with a wrong formula, unrelated to the atom model, while the illustration describes the naïve- (trajectory based) model of the atom, and does not account for the orbitals structure.</p>
<div style="text-align: center;">  </div> <p>(Undergraduate student)</p>	

Visual conceptual model: *Energy levels are 'layered areas' in which the electrons are occupied. Each energy level has a number, which expresses its distance from the nucleus, the number of electrons it can occupy, and its orbitals. In older models of the atom the energy levels were described as follows →*
But today it is known (or at least assumed) that the

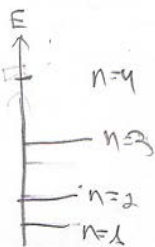


electrons are not in a "trajectory" but rather in an area in which there is a certain probability for them to be found.



(High school student)

Mathematical model: *The state of the particle can be described by a specific model which determines its energy levels. The energy level in which the particle is found is determined by the orbital in which the particle is found - n. For example for a single particle in a potential well the energy level is*



$$E_n = \frac{n^2 h^2 \Pi^2}{2mL^2}$$

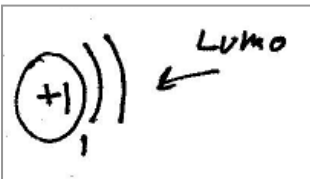
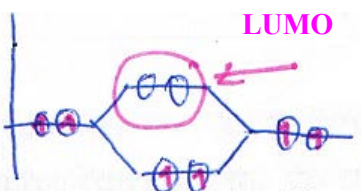
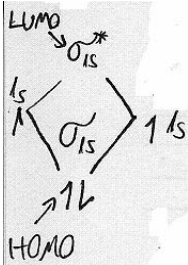
(Undergraduate student)

The student explains the shift from previous trajectory based model (which appears in the upper illustration) to the visual-conceptual quantum mechanics model that was taught in the module. Both his illustration of a dot -diagram of p orbital, and the textual explanation describe the probabilistic nature of the orbital. Yet, the student confuses the terms and regards the 'main quantum number' with 'energy level'.

The student presents correctly the generic mathematical structure of the quantum mechanics theory for the energy level concept, which he learned in his academic chemistry courses. He gives as an example the equation for energy levels of a single particle in a potential well. This model is not introduced to honors students in the module.

Understanding concepts related to the electronic structure of molecules. Learning the electronic structure of molecules includes the concepts of bonding and anti-bonding molecular orbitals, as well as HOMO and LUMO orbitals (the highest occupied molecular orbital and the lowest unoccupied molecular orbital, respectively). In Table 3 we present examples of high school and undergraduate student responses to the post-questionnaire assignment of describing the LUMO concept visually and textually. The answers revealed different stages of understanding the concept: misconception based on naïve model, partial understanding, and full understanding of the concept as taught in the module.

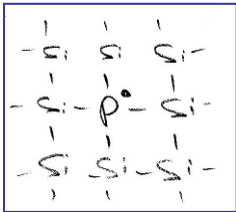
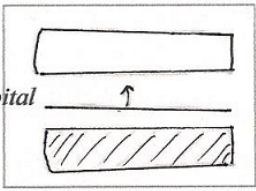
Table 3 Response of students to the description of the LUMO orbital concept

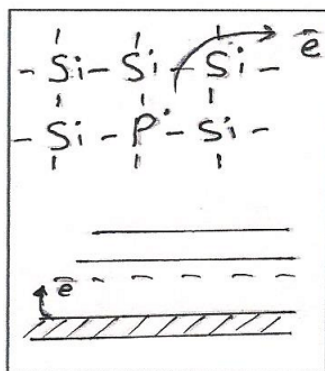
Students' response	Analysis
<p data-bbox="181 268 470 304"><u>An incorrect response</u></p> 	<p data-bbox="711 268 1435 493">The student presents a naïve model of trajectories, and not of orbitals. The illustration presents a hydrogen atom, not a molecule. It seems that he only understood the part of the definition explaining that this is the lowest unoccupied orbital, but did not grasp that these are molecular orbitals.</p>
<p data-bbox="181 520 479 556">(High school students)</p> <p data-bbox="181 562 479 598"><u>Partly correct response</u></p> <p data-bbox="181 630 698 735"><i>LUMO orbital: This is the unoccupied orbital located at the lowest energy level. For example:</i></p> 	<p data-bbox="711 562 1435 1039">The student presents a diagram the molecular orbitals levels and adds a correct explanation of the concept. The diagram of energy levels corresponds to the quantum model and presents the formation of molecular orbitals from atomic orbitals. However, it contains inaccuracies. There is no indication in the figure, which are the atomic orbitals the student refers to. If the orbital is of the s type, there should be 1 atomic orbital and if the orbital is of the p type there should be 3. Instead, there are 2 atomic and 4 molecular orbitals. Moreover, the number of electrons in the atomic orbitals (4) does not match the number in the molecular orbitals (2).</p>
<p data-bbox="181 987 462 1022">(High school student)</p> <p data-bbox="181 1060 446 1096"><u>High level response</u></p> <p data-bbox="181 1102 698 1428"><i>This is the lowest unoccupied molecular orbital. It is located one level above the HOMO, the highest occupied molecular orbital. When several atoms are bound in covalent bonds their atomic orbitals "merge" to form a molecular orbital that is occupied by electrons, similar to the atomic orbital</i></p>	<p data-bbox="711 1060 1435 1354">The student describes the two orbitals, LUMO and HOMO, and explains how they are formed from atomic orbitals. His answer shows his clear understanding that the expression that the orbitals "merge" is qualitative rather than literal (therefore he added the quotation marks). His schema describes the system of the orbitals in a hydrogen molecule and includes chemical symbols of atomic and molecular orbitals.</p>
 <p data-bbox="181 1705 495 1738">(undergraduate student)</p>	

Understanding the electronic structure of the solid state. The module explains the electronic structure of lattices in terms of the characteristics of their conduction – concepts that characterize the electronic structure of insulating materials, conductive materials, and semi-

conductive materials. The concepts of valence, conduction bands, forbidden band gap, and principles of semiconductor structure are taught with reference to two semiconductor types: type N and type P. The post-questionnaire included assignments regarding the concept of the type N semiconductor. Here, too, the answers revealed different stages of understanding, as shown in Table 4. Most of the students who chose to explain this concept described it according to the quantum model taught in the module, while some described it at the micro level of chemistry understanding.

Table 4 Response of students to the description of the concept N type semiconductor

Students' response	Analysis
<p data-bbox="181 588 795 630"><u>A micro-level description</u></p> 	<p data-bbox="828 588 1437 861">The figure includes the atoms in the crystal, covalent bonds, and an unpaired electron that enables conduction on this type of semiconductor. This description is correct, but it does not represent the quantum model taught in the module for describing conduction on type N semiconductors.</p>
<p data-bbox="181 882 795 934">(High school student)</p>	
<p data-bbox="181 966 795 1008"><u>A quantum-mechanical description</u></p> 	<p data-bbox="828 966 1437 1239">In this illustration the student describes the concept using the quantum model; there are valence and conduction bands, and another orbital, created by the process of doping. In addition, an arrow marks a possible transition of an electron. Although the location and description of the orbital are not precise, the illustration demonstrates understanding of the qualitative quantum model taught in the module.</p>
<p data-bbox="181 1260 795 1312">(High school student)</p>	

Micro and quantum-mechanical description

A lattice of Si atoms (or another element from Column 4) that has undergone doping by another element from Column 5. The remaining free e creates an additional orbital at a forbidden band gap, which reduces the band gap, thus enabling conduction.
(High school student)

The upper part of the figure reflects a detailed micro level model, where the arrow describes the possible movement of the additional electron in a state of electric conduction. The drawing on bottom reflects the quantum model. Here, too, the transition of the electron is described by an arrow. The textual part of the answer also includes a combination of the micro and quantum levels.

The components of the drawing are nearly correct (the arrow is misplaced in the bottom plot), and the answer also expresses a misconception that the electrons create the orbitals (while according to quantum mechanics, the orbitals are created and the electrons occupy them). Despite these inaccuracies, the student's answer reflects understanding of the concept according to the quantum model, and he connects it to the micro and macro levels of electric conduction. The student describes the concept using two levels of understanding, micro and quantum, as two complementary models for the same concept.

The qualitative analysis presented in Tables 2 through 4 has shown that students' perception of models related to quantum mechanics consisted of different types of models, ranging from naïve models to complete quantum mechanics models. Next, we present the quantitative analysis regarding textual and visual chemical understanding and students' integration of the different levels of chemistry understanding.

Textual and visual chemical understanding – Quantitative Analysis

Textual and visual chemical understanding skills express students' understanding related to quantum mechanical content, and their ability to describe and explain these concepts using visual and textual modes. In this section we present findings related to textual and visual chemical understanding of the various research participants. The quantitative analysis included three comparisons: (1) between high school honors and undergraduate students, (2) between high school and undergraduate students who studied the module, where the high school students included high and intermediate academic level honors students, while the undergraduates were the ViCo (Visual-Conceptual)-oriented undergraduate students, and (3) the undergraduate ViCo-oriented students (who studies the module) and the undergraduate math-oriented students (who did not study the module).

High school honors vs. undergraduate students. Analyzing students' textual and visual chemical understanding average scores indicated that both honors and undergraduate students significantly improved their ability to describe concepts by using visual and textual modes and moving across them (see Fig. 1; Honors students: $t=10.57$, $p<0.0001$; Undergraduate students: $t=5.39$, $p<0.0001$). Honors students pre-questionnaire scores were lower than undergraduate pre-

questionnaire scores, but they gained more, and their post-questionnaire scores were higher. Significant difference was found between the net-gain scores (post- minus pre-questionnaire scores) in favor of the honors students ($t=2.57$, $p<0.05$)

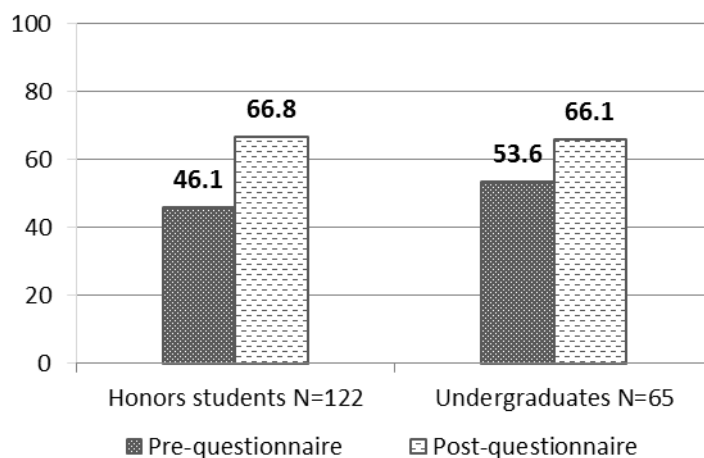


Fig. 1 Textual and visual chemical understanding mean scores of high school and undergraduate students

High school vs. undergraduate students who studied the module. Using ANOVA test, we compared the net-gains (post- minus pre-questionnaire scores) of the sub-groups of students who studied the module. We found significant difference between the sub-groups, ($F_{(2,143)}=6.12$, $p<0.01$; see Table 5). Post-hoc tests indicated that high-level honors students' net-gain was significantly higher than that of the intermediate honors students ($p<0.005$). High-level honors students' net-gain was also higher than that of the ViCo-oriented undergraduate students with borderline significance ($0.05<p<0.1$).

Table 5 Net-gain scores of textual and visual chemical understanding of high-level honors, intermediate-level honors, and ViCo-oriented undergraduate students

Sub-groups	N	Net-gain	S.D.
High-level honors	73	26.5	21.2
Intermediate-level honors	39	13.8	19.5
ViCo-oriented undergraduates	34	17.4	17.5

We examined the distribution of chemistry understanding levels that high school and undergraduate students' used in their answers. The responses demonstrate mainly micro and quantum level understanding. We counted and added up the levels of understanding revealed in all three assignments and calculated the frequencies in the pre- and post-questionnaires. The N items were distributed across the micro, quantum, and micro + quantum chemistry understanding levels. Fig. 2a and Fig. 2b present this distribution in pre- and post-questionnaires, respectively,

by sub-groups: high-level, N=73, and intermediate-level, N=39² honors students, and ViCo-oriented undergraduate students, N=34).

Findings in Fig. 2a. indicate broad differences between the sub-groups of students in the pre-questionnaire. The answers of the intermediate-level honors students were mainly on the micro level, with little use of the quantum level. The same picture was apparent among the high-level honors students; however, the quantum level already appeared. Among the ViCo-oriented undergraduate students, the quantum level already appeared in their answers on the pre-questionnaires (see Fig. 2a), probably since these students had studied the course, Basics of Chemistry, a year or two earlier.

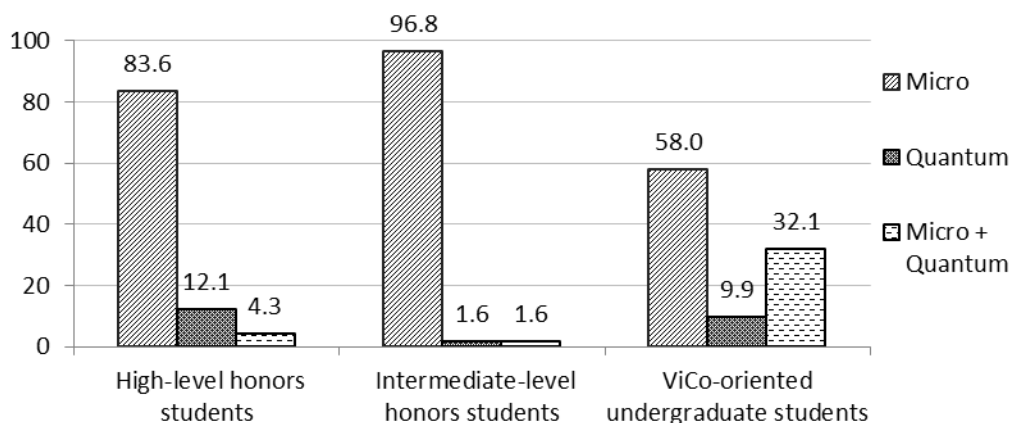


Fig. 2a

Distribution of chemical understanding levels – pre-questionnaire

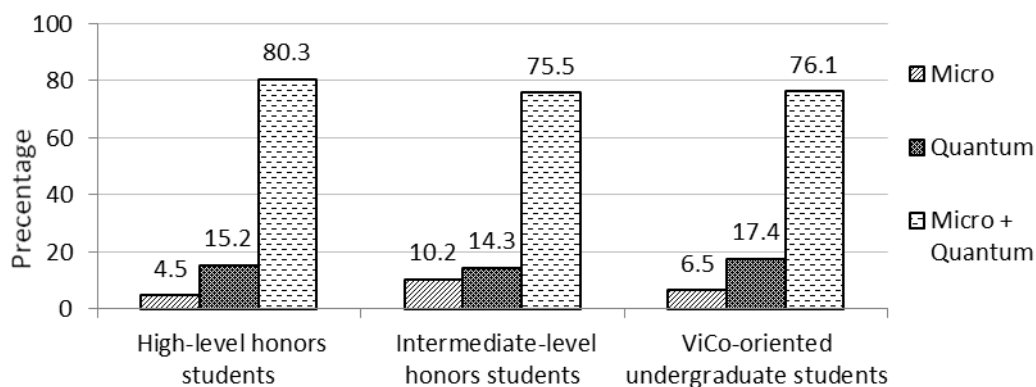


Fig. 2b Distribution of chemical understanding levels post-questionnaire

In the post-questionnaire, the number of items increased in all sub-groups and the highest frequency was that of a combination of the micro and quantum levels. High school honors and

² N=112 in the honors sub-groups due to missing teachers' grades which were needed in order to assign each student to a sub-group

undergraduate students minimized the gap between them in terms of the integration of micro + quantum levels in their answers. High-level honors students had a higher frequency in integrating the micro + quantum levels than intermediate-level honors students.

Graduate ViCo-oriented vs. graduate math-oriented students. In order to find out which variables affect the post-questionnaire scores of the undergraduate students in textual and visual chemical understanding, multiple regression analysis was carried out. The regression was significant with respect to the variables we measured – pre-questionnaire, enrichment type and faculty ($F_{(3, 54)}=13.56$, $p<0.000$). Pre-questionnaire was the most significant variable ($t= 3.90$, $p<0.0001$). Participation in the ViCo-oriented enrichment ($N=34$) increased the standard (Z) score of these undergraduate students by 0.32 in comparison to their math-oriented enrichment ($N=24$) peers ($t=3.02$, $p<0.01$). Students from the Chemistry Department had 0.23 higher standard (Z) scores than students from other faculties ($t=2.18$, $p<0.05$).

Discussion

The *Chemistry – From “the Hole” to “the Whole”*: *From the Nanoscale to Microelectronics* module focuses on teaching quantum mechanical topics to honors students using a visual-conceptual approach, which is contrasted with quantitative, classic approach for teaching most of the undergraduate quantum chemistry courses. In addition to implementing and assessing the module in high school, it was also partially implemented and assessed in an undergraduate quantum chemistry course.

The four evolutionary stages of understanding quantum mechanics

The qualitative analysis reflected four evolutionary stages of understanding quantum mechanics, as presented in Fig. 3.

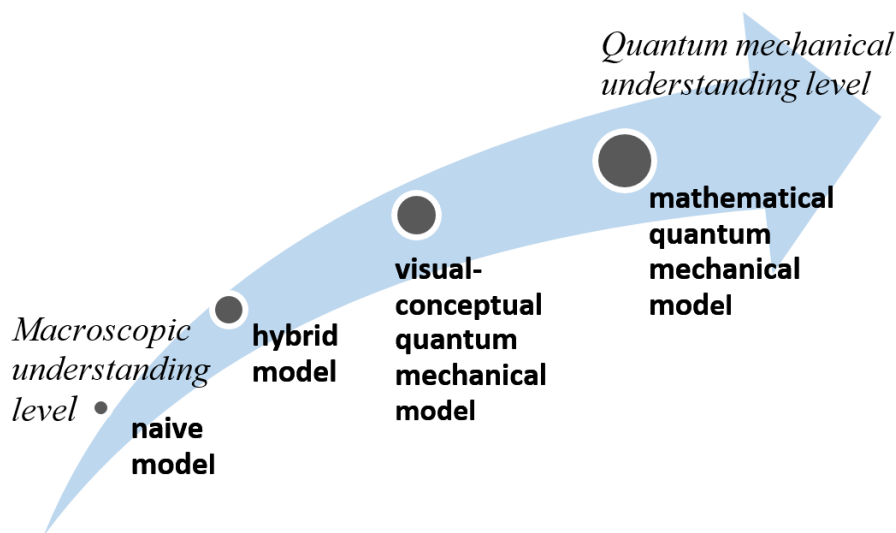


Fig 3. Developmental stages of students' chemical understanding in quantum mechanics

Naïve models, such as the planetary or solar system model (Harrison and Treagust, 1996; Stevens et.al, 2010, Taber, 2001a), are based on a macroscopic perspective that describes electron rotation in a deterministic trajectory around the nucleus, resembling that of a planet rotating around the sun. In our qualitative analysis we discovered students' use of hybrid models

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2
3 that mix the terminology of definite orbits of the electron with the probabilistic quantum
4 mechanical concept. We also discovered the use of a hybrid model using a mathematical
5 formula.

7 These findings are consistent with those of previous studies, which indicated that honors and
8 college students merge concepts from previous historical models with probabilistic quantum
9 mechanical terminology (Mashhady and Woolnough, 1997; Stefani and Tsaparlis, 2009; Stevens
10 et.al, 2010; Taber, 2002, 2005; Papaphotis and Tsaparlis, 2008).

11 The visual-conceptual quantum mechanics model, which was taught in the module, is more
12 abstract and required understanding of the quantum level. Honors students restricted their
13 explanations to qualitative and visual terms, which they had learned in the module. Some of the
14 undergraduate student responses referred to the generic mathematical structure of quantum
15 mechanics theory, based on their background knowledge (see Fig. 3).

16 Historical reconstruction of the atomic model, taught as part of most chemistry and physics
17 curricula, may be a source of confusion to some students. Students need to understand why
18 previous models do not represent the acceptable atomic quantum model, which scientists believe
19 is more accurate. Although some researchers question the need to teach quantum mechanical
20 concepts in secondary school and introduction courses in college (Tsaparlis, 1997; Gillespie,
21 1991, 1996), to this end, we recommend that high school students, as well as students in college
22 introductory chemistry courses, will be gradually exposed to ever more sophisticated models,
23 culminating in the quantum mechanics model. This approach is in line with recommendations
24 suggested by researchers in previous studies (Shiland, 1997; Coll et al., 2005; Niaz and Coştu,
25 2009; Stevens et.al, 2010), some of whom recommended teaching students the different models,
26 emphasizing their limitations and advantages.

31 **Textual and visual chemical understanding**

32
33 The quantitative analysis has shown that students in our study improved their textual and visual
34 chemical understanding skills. However, the extent of the high school students' improvement
35 (net-gain) was significantly higher than that of the undergraduate students. These results might
36 relate to the shorter duration of the enrichment course to which the undergraduate students were
37 exposed. The higher mean scores of undergraduate students in the pre-questionnaire compared
38 with the honors students is due to the more extensive experience of the undergraduate students in
39 using visual representations and better understanding of quantum mechanical concepts, which
40 they had gained in previous physical chemistry courses. This relatively higher starting point may
41 also explain their lower improvement.

42
43 In this research, we started evaluating the students' understanding of chemistry via four
44 chemistry understanding levels – macro, micro, symbol and process – using a method developed
45 in earlier research for evaluating textual responses (Dori and Sasson, 2008; Kaberman and Dori,
46 2009). Analyzing the students' responses, the need to add a fifth level of understanding – the
47 quantum level – became apparent. This level includes the ability to depict the electronic structure
48 of atoms, molecules and solid state in terms of quantum mechanics theory. After learning the
49 module, there was a shift in the honors students' responses from the micro chemistry
50 understanding level to the quantum level and to the combination of the two. This might indicate
51 that most of them had gained better understanding of the quantum model of atoms and molecules
52 while studying the module.

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55 Our findings also strengthen the claim of Tasker and Dalton (2006) that textual and visual modes
56 should be intertwined in order to promote conceptual understanding. The findings are consistent
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3 with the argument of Gunel and colleagues (2006) that visualizations enable the construction of a
4 richer conceptual understanding of a set of quantum mechanical topics.

5
6 However, these findings contradict those of Papaphotis and Tsapalis (2002, 2008), who claimed
7 that most of the honors students failed to attain understanding of the probabilistic nature of
8 atomic orbitals and retained a deterministic perspective. The differences between their study and
9 ours might be related to the differences in the teaching approach of the new module, which is
10 less mathematical-oriented approach. The definition of honors in the two countries might be
11 another explanation to the differences in findings between the two studies.
12

13
14 Textual and visual chemical understanding skills of the undergraduate students, who studied the
15 module as enrichment, was significantly higher than their math-oriented peers. This finding
16 points to the benefit that undergraduate students, who had been exposed to the module, gained by
17 improving their conceptual understanding of quantum mechanical concepts and their ability to
18 apply visual and textual modes to explain and describe quantum mechanical concepts. Our
19 finding is consistent with those of Kalkanis and colleagues (2003), and Cataloglu and Robinett
20 (2002), who found that implementation of a qualitative teaching approach, which integrates
21 conceptual and visual understanding in a quantum mechanics course, improved students'
22 understanding. Based on our findings and those of others, we recommend integrating the visual-
23 conceptual approach into both high school and undergraduate quantum chemistry courses in
24 particular and into physical chemistry curricula in general.
25
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27 28 **Limitations and strengths of the research**

29
30 Our research had some limitations. One was that we could not find a comparison group for the
31 honors students, because the topics of the module had not been taught in Israel before. Honors
32 students do not have sufficient background in mathematics for learning quantum mechanics.
33 Therefore, we based our module on visual-conceptual explanations. Another limitation is that the
34 undergraduate students were only partially exposed to the module, and the exposure was for a
35 short duration. A future study may investigate the effect of longer exposure to this qualitative
36 approach. Despite these limitations, the qualitative aspect of the assessment method is valuable
37 for a variety of topics in chemistry and science in general.
38

39
40 The research findings indicated that using a visual-conceptual approach to teaching quantum
41 mechanical concepts and principles and their integration into daily life applications may help
42 overcome the need to introduce mathematical aspects of quantum theory to honors students. The
43 combination of these aspects is a novel element in our research. Most of the honors student
44 responses after studying the module demonstrated a level of quantum mechanical understanding
45 that enabled them to clearly explain the main concepts in this area.

46
47 Our module emphasized the link between quantum-mechanics theory and daily life phenomena,
48 such as the color of pigments and the transition of metal from a conductor to a semi-conductor.
49 Using terms of orbitals, valance and conducting bands, which arise from quantum mechanics
50 theory, enabled the students to understand how microelectronic devices, such as LED (light
51 emitting diode), work without teaching them the mathematical background they lacked. These
52 kinds of daily life applications, which are not represented in most chemistry textbooks (Shiland,
53 2007), may help students recognize the usefulness of quantum mechanics theory and make it
54 easier for them to shift from the previous models they possess to the quantum model (Stevens et
55 al., 2010). We also found that embedding a visual-conceptual approach in an undergraduate
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3 quantum mechanics course broadened students' views and conceptual understanding of key
4 quantum mechanical terms.

5 One theoretical contribution of this study is the addition of the quantum level as a fifth level of
6 chemistry understanding, augmenting the current set of four chemistry understanding levels –
7 macro, micro, symbol and process. In addition to being a means to understand and explain
8 chemistry, this level provided the basis for our self-developed assessment tool enables evaluating
9 chemistry understanding in both visual and textual modes. Drawings and illustrations were
10 applied for assessing students' understanding of the atomic structure and chemical bonding (Coll
11 and Treagust, 2003; Harrison and Treagust, 2000; Stevens et al., 2010; Wheeldon, 2012). The
12 tool we developed contains rubric for analyzing and scoring scientific drawing and illustrations
13 (see Appendix 2) designed specifically for assessment of quantum mechanics topic
14 understanding, and to the best of our knowledge is the first and so far only such tool. This tool
15 enables characterization of students' chemical understanding of phenomena, such as
16 semiconductors, which can be described at the micro level by illustration of covalent bonds and
17 "holes" (García-Carmonaa and Criado, 2009) or by using quantum-mechanical concepts, such as
18 valance and conducting bands, which constitute the quantum basis of the phenomena. While
19 tailored to quantum mechanics understanding, this tool can be adapted in other research in
20 chemistry, as well.

21 This research contributes to the body of knowledge on visualization and thinking skills in
22 chemistry, and could potentially enhance the teaching and learning of quantum mechanical
23 concepts at both the honors and undergraduate levels. From the practical perspective, the
24 research may help curriculum developers and teachers to incorporate visual representations in the
25 design and assimilation of new learning materials on the structure of matter at the nanoscale
26 level.

27 Finally, the approach studied in this work has an additional value in the broader context of
28 chemistry studies. In many fields of chemistry (though not in theoretical quantum chemistry), a
29 visual-conceptual approach is commonly followed. For example, orbitals are discussed in the
30 context of organic reactions mechanisms, at a level, which is far from the formal way taught in
31 undergraduate courses, and from the scope of rigorous mathematical models. Therefore, beyond
32 being an evolutionary stage towards a more rigorous theoretical understanding, the qualitative
33 understanding of quantum mechanics models and concepts, as pursued here, provides a practical
34 thinking tool for all chemists

35 36 37 38 39 40 41 42 43 **References**

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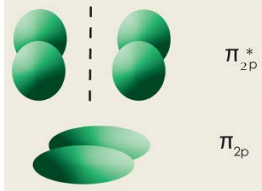
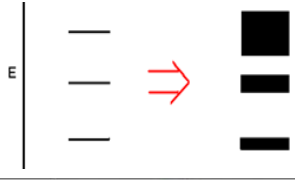
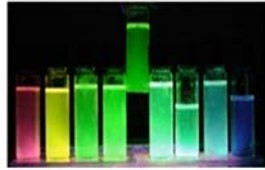
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Appendix 1 - Table 1

The characteristics of the module *Chemistry – From “the Hole” to “the Whole”*: From the Nanoscale to Microelectronics

Topics	Key Concept	Applications	Visualizations
The electronic structure of atoms	Atomic orbitals, energy levels, emission spectrum	Pyrotechnic, the firework colors	
The electronic structure of molecules	Molecular orbitals: Bonding, anti-bonding, HOMO, LUMO	Why do organic pigments have colors? stick lights	
The electronic structure of solid state	Energy bands, N and P type semiconductors	Microelectronic of solid state apparatus, light emitting diode	
*Quantum size effect application	Observable size-dependent characteristics of nanoparticles	Tunable emission from CdSe based nanocrystals of different sizes, carbon nanotubes	

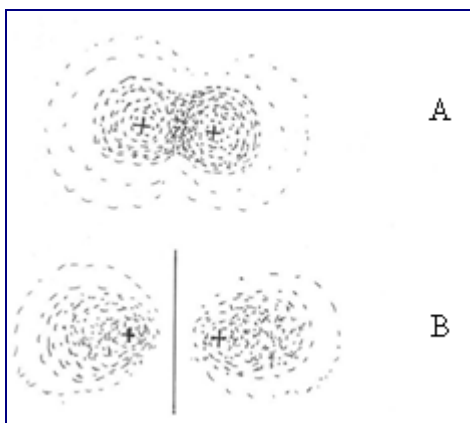
*The picture was taken by Dr. Roni Costi at Prof. Uri Banin's lab, the Institute of Chemistry and the Center for Nanoscience and Nanotechnology, The Hebrew University of Jerusalem, Jerusalem, Israel

Appendix 2 – Assignment C

The Figure below represents a two dimensional model of molecular orbitals. Illustration A and illustration B represents the orbitals of a di-atomic molecule. Each illustration refer to a different molecular orbital.

Please explain the illustration in the Figure by answering the following questions:

- i. What do the "+" symbols represent?
- ii. What does the vertical line in illustration B stand for?
- iii. What does the density of the dots in the illustration represent?
- iv. Assuming that the two orbitals are formed from the same two atomic orbitals, which one has a higher level of energy? Please explain.



A two dimension model of molecular orbitals

Appendix 3 – Assessment tool and rubric for assignments A, B, and C

Assignment	Representation type	Category	Explanation and corresponding score	Max score
Assignments A and B	Visual	Number of illustrations	No illustration – 0	3
			One illustration – 1	
			Two illustrations – 2	
		Two illustrations that are connected to each other – 3		
		A naïve illustration – 1		
	Character of illustrations	An illustration that focuses on the micro level – 2	3	
		An illustration that focuses on the quantum mechanical level – 3		
	Correctness	An improper or erroneous illustration – 0	2	
		A partially correct illustration – 1		
	A correct illustration – 2			
Complexity	An illustration with one item – 1	3		
	An illustration with 2-3 items – 2			
An illustration with 4 items or more – 3				
Textual	Correctness	No explanation, or a wrong one – 0	2	
		A very short or partially correct explanation – 1		
	A correct and detailed explanation – 2			
	Chemistry understanding levels	The number of chemistry understanding levels out of the symbolic, macroscopic, microscopic, process, and quantum mechanical levels, (none of the answers included more than 3 levels)	3	
Match between the two modes	Coherence	There is no correct match between textual and visual representation – 0	1	
		There is a correct match between the two modes of representation – 1		
Assignment C	Textual	Correctness and detailed content	Each sub-question was scored between 0-2 with respect to its correctness and levels of details	4*2=8
		Chemistry understanding levels	The number of chemistry understanding levels out of the symbolic, macroscopic, microscopic, process, and quantum mechanical levels, (none of the answers included more than 3 levels)	3

* Only correct and relevant items were counted