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Inquiry-Based Activities and Games That Engage Students in Learning Atomic Orbitals

Xiao Li, Marc Muñiz, Karlun Chun, Jonathan Tai, Francesca Guerra, and Darrin M. York*

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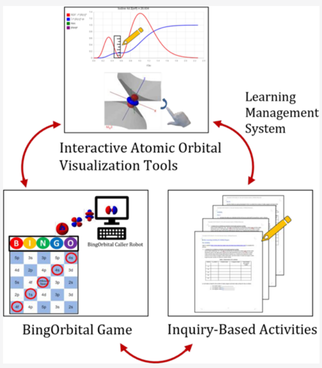
ABSTRACT: Atomic orbitals represent an essential construct used to develop chemical bonding models, upon which other more advanced chemistry topics are built. In this article, we share a series of active-learning activities and a gamified approach to develop students' representational competence about atomic orbitals and to engage students in learning the properties of atomic orbitals. These properties are essential for understanding an array of fundamental concepts such as penetration and shielding, relationships such as periodic trends, and models used to describe chemical bonding. The activities employ an inquiry-based approach to engage students in exploring the relationship between atomic orbitals' spatial properties and quantum numbers. The activities guide students to collect data to verify periodic trends and construct electronic configurations. The activities utilize Orbital Explorer Web site for visualization, comparison, and analysis of atomic orbitals. The Orbital Explorer Web site is described in a related Technology Report. The activities and the game are suitable to be conducted in both in-person and remote-teaching settings.



KEYWORDS: *First-Year Undergraduate/General, Atomic Properties/Structures, Inquiry-Based/Discovery Learning, Internet/Web-Based Learning*

1. INTRODUCTION

Atomic orbitals are fundamental constructs used as a foundation from which theoretical models for chemical bonding[1] are built and present conceptual difficulties for many students.[2] The concepts of atomic orbitals and electron configurations are generally introduced in early chapters of the general chemistry curriculum and reviewed again in early chapters of organic chemistry. The first and second big ideas, "Atoms" and "Bonding", on the ACS Anchoring Concept Content Map (ACCM)[3,4] for both general[3] and organic[4] chemistry, present important content centered on atomic orbitals and electron configurations (Table S1 in the Supporting Information). Atomic orbitals, which are modeled as solutions to the Schrödinger equation of hydrogenic atoms with orbital-dependent effective nuclear charges, are abstract quantum mechanical concepts and are often challenging for undergraduate students to learn and master.[5] Electron configurations is essential in predicting atomic properties and how an atom forms chemical bonds with other atoms in a molecule.[1] Rote-memorization of rules (e.g., Madelung's rule) causes misconceptions and hinders students' deep understanding of the electronic structure of atoms.[6−8] In order to assist students in learning the essential and complex conceptual knowledge of atomic orbital and electron configuration effectively, a series of activities, a gamified design, and an accompanying visualization tool suite[9] have been developed, guided by recent educational research findings.[10−12] The activities adopt inquiry-based learning (IBL) approach,[11] and the game is designed as a retrieval practice.[12] IBL has been demonstrated to improve student outcomes and narrow achievement gaps,[13,14] enhance conceptual understanding,[10,15] and facilitate teaching deep conceptual knowledge.[16] Retrieval practice has been demonstrated to be important for long-term retention[17] and serves as an effective tool to promote conceptual learning.[12] The pedagogical structure of activities and tools, their implementation, and results are elaborated in the following sections.

2. INQUIRY-BASED LEARNING ACTIVITIES

2.1. Components

We share and introduce a learning resource package containing two activity worksheets and a game in this article (Figure 1). The two activities are Activity 1 − *Atomic Orbital Shapes* and Activity 2 − *Periodic Properties and Electron Configurations*. Activities 1 and 2 are designed to be conducted in sequence. The game is called *BingOrbital*, whose invention is inspired by the well-known Bingo game. The activities and game's Web site is called *Orbital Explorer*, which contains two interactive visualization tools: Tool 1 − *Atomic Orbital Explorer* and Tool

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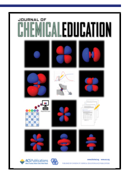

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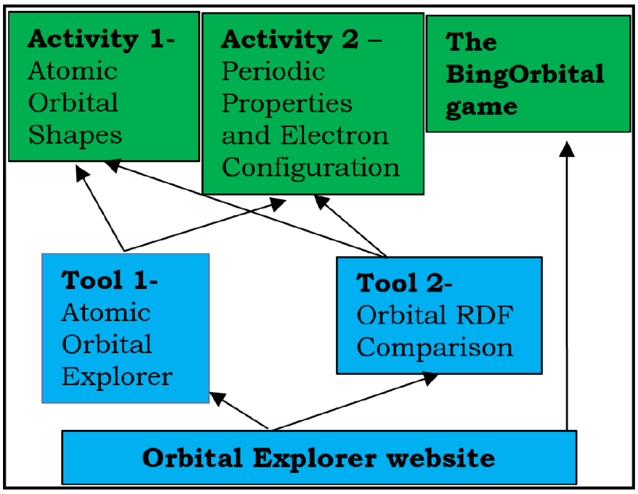

Figure 1. Scheme showing the components of the learning resources shared by this contribution and how they are interrelated. Activities and game are displayed in green boxes, and web-based tools are displayed in blue boxes. The arrows indicate how the web tools support activities.

2 − *Orbital RDF Comparison*. The Orbital Explorer Web site: elearning.rutgers.edu/orbitalexplorer.

In Activity 1, students study atomic orbitals by exploring the three-dimensional orbital isosurface and radial distribution function (RDF) plot with tool 1 and develop mathematical expressions of the number of radial and angular nodes in terms of quantum numbers. Students observe the relationship among orbital size, the number of radial nodes, and the effective nuclear charges with tool 2. Students use the collected data and derived models to rationalize how the number of radial nodes influences the atomic sizes and leads to penetration and shielding effects that affect the atomic orbital energies. In Activity 2, students practice writing electron configurations by applying the Aufbau principle and solve a jigsaw puzzle by applying knowledge of periodic trends. Furthermore, students are guided to explore atomic orbital energies and practice writing electron configurations for transition-metal cations. Through Activity 2, students gain insight into the use of atomic orbitals and their related diagrams, including realizing some common misconceptions (e.g., orbital energy ordering is a "rigid ladder"[7]), to make practical predictions. The learning objectives and the aligned ACCM content are listed in Table 1.

The worksheets can be printed as handouts and distributed to students if the activities are conducted with paper and pencil. In remote instruction, the activities can be distributed electronically as PDF files. The word and PDF files of Activity 1 and 2 worksheets (the recommended 2021 version and previous versions as references) and the associated keys are included in the Supporting Information. In addition, the two activities are also made available as Modules on Canvas, a widely adopted learning management system (LMS) for automatic collection and grading. The instruction on importing learning resources to a course site on Canvas is provided in the Supporting Information.

2.2. Design Ideas

The activities employ an inquiry-based learning (IBL) approach. A definition synthesized from literature characterizes IBL as a learning approach in which students learn knowledge through the investigation into data or information to answer questions or solve problems.[11] Inquiry-based learning (IBL) is part of a broader set of pedagogical approaches referred to as active learning: approaches that directly engage students in meaning-making activities rather than expecting them to passively absorb information. Meta-analyses on active learning

Table 1. Desired Student Learning Outcomes with the Aligned Contents on ACS General Chemistry Anchoring Concept Content Map (ACCM[3])

activity	learning objectives	indexes of aligned ACCM[3] contents[a]
Activity 1	1. Formulate a model for the number of radial nodes and number of angular nodes as a function of the principal and angular momentum quantum numbers, n and l, respectively.	I−B2a,b; X-D
	2. Apply the model to predict:	I−B2a,b
	(1) the number of radial and angular nodes for any atomic orbital.	
	(2) the trend in how the number of radial and angular nodes changes as the principal quantum number *n* increases for a series of orbitals with fixed angular momentum quantum number *l* (e.g., 3*d*, 4*d*, 5*d*).	
	(3) the trend in how the number of radial and angular nodes changes as the angular momentum quantum number *l* increases for a series of orbitals with fixed principal quantum number *n* (e.g., 4*s*, 4*p*, 4*d*).	
	3. Observe how orbital size changes with the principal and angular momentum quantum number.	I−B2a,b
	4. Rationalize, in terms of nodal structure (number of radial and angular nodes), how changes in the principle and angular momentum quantum numbers will affect the atomic orbital size and shape.	I−B2a,b
	5. Identify trends in degree of shielding and penetration of atomic orbitals in a given element in the second period, rationalize the origin of sp degeneracy in terms of degree of shielding and penetration.	II−E1c
	6. Identify the periodic trend in 2s-2p energy splitting, rationalize how the energy splitting affects sp mixing (hybridization), and apply trends and rationale to make predictions about energy cost of sp hybridization for second row elements B, C, N, O and F.	I−C2a
Activity 2	1. Write full and condensed electron configurations for neutral atoms and ions (s-, p- and d- blocks) applying Aufbau principle, Pauli's exclusion principle and Hund's rule.	I−B3a,c
	2. Predict and explain the trend of periodic properties (electron affinity, ionization energies, electronegativity, etc.) in term of electronic structure.	I−C1a,b,c;
	3. For transition metals (d-block), construct atomic orbital energy diagram from orbital energy data to verify or falsify Madelung order. Write electron configurations for transition-metal ions by removing the most energetic electrons from the neutral-atom configuration.	I−B3b
BingOrbital	1. Practice recognizing atomic orbitals by shape and nodal properties	I−B2a,b; X-D

[a]Content coverage by the activities on ACCM[3] is summarized and organized in Table S1 in the Supporting Information.

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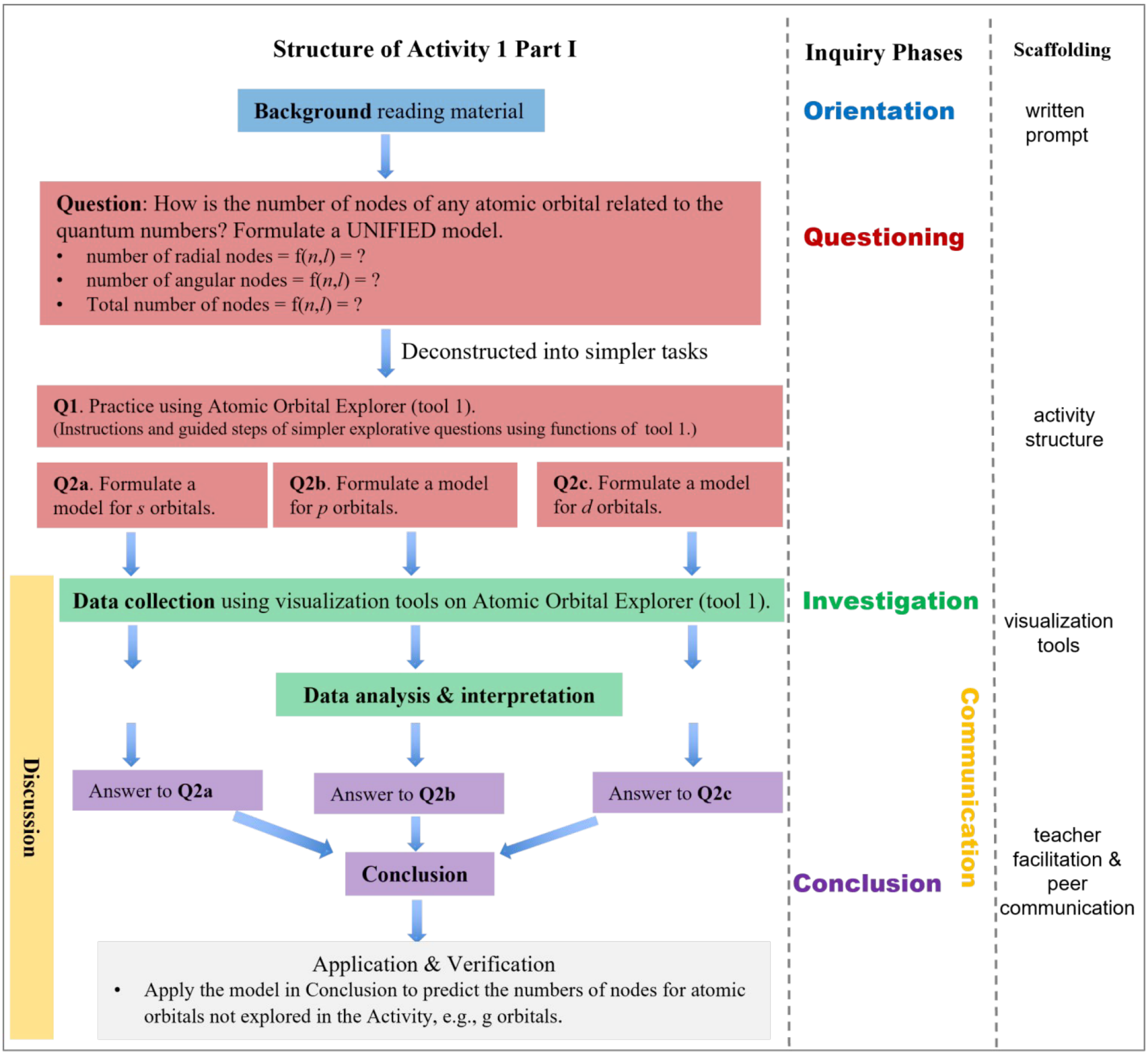

Figure 2. Design model for Activity 1 Part I. The anatomy of the activity is displayed in the left column. Activity subunits serving the same function in the inquiry cycle[19] are highlighted according to a color code: Orientation − Blue, Questioning − Red, Investigation − Green, Conclusion − Purple, Communication − Orange. The names of the corresponding inquiry phases are displayed in the middle column and are colored according to the same color code as the left column. The types of scaffolding provided to students during the activity are indicated in the right column. The most important type of scaffolding[20,21] for a particular phase is placed near the related phase. However, most scaffoldings, especially teacher facilitation, are available throughout the whole inquiry cycle. Teacher facilitation includes facilitation provided by both instructors and teaching interims[22] in the actual implementation.

suggest that when such approaches are meaningfully integrated into undergraduate STEM classroom environments, student outcomes improve and achievement gaps narrow.[13,14] Research findings indicate IBL poses a positive impact on students' conceptual understanding and academic skills.[10,15] It is argued that inquiry-based learning is effective in teaching deep conceptual knowledge[16] compared to direct instruction.[18]

The structure of Activity 1 Part I is analyzed as an example to demonstrate the inquiry-based design (Figure 2). A typical IBL activity proceeds in the following phases: *orientation*, *conceptualization* or *questioning*, *investigation*, *conclusion*, and *discussion*.[19] The Activity begins with an *orientation*[19,23] or *engagement*[24] phase in which the topic of the Activity is introduced. Students read the two-page background material about the quantum theory of atomic orbital in this phase. Next is a *conceptualization* phase, which comes in two major variations: *questioning* or *hypothesis generation*.[19,23] This phase (highlighted in red in Figure 2) in Activity 1 Part I presents a question to be investigated instead of a formula to be tested, so it is labeled as the *questioning* phase. The Activity asks for the mathematic relationship between the number of nodes (radial and angular) and quantum numbers. This relatively complex question is broken down into one task that familiarizes students with tool 1 and three simpler subquestions each focusing on *s*, *p*, or *d* orbitals to lead students step-by-step to reach the complex question. After being introduced to the

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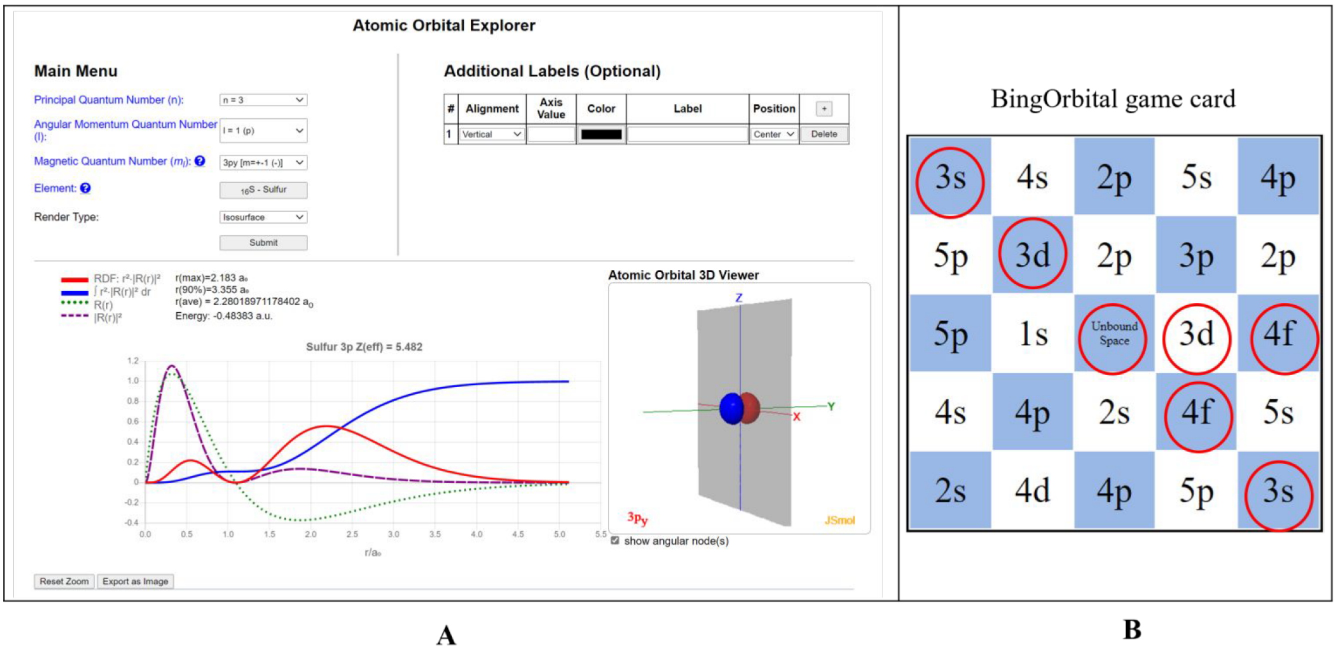

Figure 3. Screenshot of the (A) Atomic Orbital Explorer and (B) BingOrbital game card. A detailed technical presentation of the Orbital Explorer and BingOrbital game is presented elsewhere.[9]

question to be studied, students enter the *investigation* phase. They are guided to collect data with Atomic Orbital Explorer (tool 1),[9] analyze data, and answer subquestions and the complex question. The *conclusion* phase follows, during which students state their answer to the scientific question, which is a generalized formula of the number of nodes as functions of quantum numbers in this case. The *discussion* phase generally contains subphases: *communication* in which students communicate their findings externally to or with peers and *reflection* in which they reflect internally on the whole IBL process. The Activity under discussion focuses on the *communication* phase. In the Activity, students are preassigned to study groups of three to four members and are instructed to present results to, and discuss questions with group members, teaching interims[22] and instructors throughout the data collection and conclusion drawing procedures. Thus, *communication* occurs synchronously with the *investigation* and *conclusion* phase. Following the resolution of the question, students are asked to apply the solution to predict the number of nodes for more orbitals and verify the predictions with tool 1. Such a phase is classified as the *application* phase, which is an additional IBL phase suggested by some literature.[25,26]

The effectiveness of the IBL approach is dimidiated if unstructured and lacking guidance to students.[27,28] Guidance and scaffolds are critical for the success of inquiry-based learning and contribute to a high fidelity of implementation.[29] Several types of helpful guidance[20,21] are written prompts, activity structure, visualization tools, and teacher facilitation. The forms of guidance provided to learners for Activity 1 Part I are indicated in Figure 2. Written Prompts are short passages of information, instruction, or reminder, and are also called "explanation"[30] or "direct presentation of information"[31] in other literature. Prompts are provided throughout Activity 1 and provide the most important guidance in the *orientation* phase. The topic of the atomic orbital is introduced to students through a short reading passage. Activity Structure,[20] termed "process constraints" in other literature,[21] is a type of scaffold that reduces the cognitive burden for novices through the deconstruction of a complex task into manageable ones. As shown in Figure 2, the complex Question is deconstructed into subtask Q1 and subquestions Q2a, Q2b, and Q2c. This way, students are led to explore the relationship between the number of orbital nodes and quantum numbers (n and l) with angular quantum number l restrained first. The Visualization/Simulation Tool is an emerging type of scaffold for IBL.[31,32] The novelty of this contribution lies in the adoption of Orbital Explorer[9] as scaffolding tools for the *investigation* phase. Students make use of Orbital Explorer[9] as a visualization tool to explore atomic orbitals and as a virtual laboratory for data collection. Teacher facilitation, dialogic[30] for this Activity, is guidance such as reminders, hints, or explanations provided by instructors and teaching interims[22] who constantly monitor the activity progress. Peer discussion is a feature of collaborative learning and is important for knowledge construction.[33,34] In past implementation, students worked in teams on the activity in face-to-face instruction and worked individually on the worksheet first and then discussed in online conference rooms in remote instruction.

Activity 1 Part II and Activity 2 are designed with similar IBL frameworks, and the design models for them are available in the Supporting Information (Figures S1 and S2).

3. ORBITAL EXPLORER AND BINGORBITAL GAME

Orbital Explorer[9] (Figure 3) is an online set of tools that enable visualization and interactive query of atomic orbitals. BingOrbital is an original chemistry educational gamification design that allows students to practice recognizing atomic orbitals based on the RDF and 3D isosurface and is applied here in conjunction with Activity 1 as a retrieval practice. Instruction for the game is provided in the Supporting Information. A detailed technical presentation of the Orbital Explorer tools and BingOrbital game and how they act synergistically with the activities to enhance learning is presented elsewhere.[9]

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4. RESULTS AND IMPROVEMENTS

The activities have been implemented for the Honors General Chemistry I course at Rutgers University since the Fall 2019 academic term. For the same course in the Fall 2018 term, an earlier version of the activities drew upon a third-party atomic orbital simulation Web site called Hydrogen Atomic Viewer.[35] Both qualitative feedback and quantitative results in 2019 are collected, analyzed, and compared to 2018. The instructional team generally found that the activities improved learning processes in 2019 compared to 2018 in the following aspects. First, the team was able to spend more time answering content-related questions from students during the activities, as they received fewer technical troubleshooting requests caused by Java installation on browsers. Second, students were able to acquire understanding of concepts such as nodal surfaces faster with the high-quality, unambiguous visual representations provided by Orbital Explorer.[9] Such an improvement was reflected in the shorter time needed by students to identify and count the number of angular nodal surfaces of given orbitals. In addition, the data collection phase became smoother as students were able to collect all types of required data (figures and numerical outputs) on the one-stop Orbital Explorer Web site instead of across platforms. In 2020, during the pandemic, the activities and web-based tools were found to be perfectly compatible for remote instruction.

Select aggregated students' exam results of specific questions for the Fall 2018 and 2019 academic terms are summarized in Table 2. An improvement in the average score of Item 2 that targets electron configuration and periodic trend is observed in 2019. The average scores of Item 1 targeting atomic orbital representational competence show no statistically significant difference. The test items are available in Table S3 in the Supporting Information.

Table 2. Students' Test Results in 2018 and 2019

	2018	2019	p-value[a]
Number of Students	84	56	NA
Item 1 Average[b] (identify atomic orbitals)	58.3(8.6)%	56.5(11.2)%	0.746
Item 2 Average (write electron configuration and predict periodic trend)	65.3(3.9)%	74.1(7.9)%	0.044

[a]Two-tail p-value for t-test of two-sample assuming unequal variances ($\alpha = 0.05$). [b]Standard deviations of the averages are shown in the parentheses immediately after the average.

This work is compared with other existing activities[36−38] targeting similar concepts (Table 3). All activities under comparison report positive results despite various analytical methods. With regard to the content and pedagogical structure, this work is advantageous compared to other activities in the following aspects. First, this work containing a series of activities covers a greater range of interrelated general chemistry topics. As the design of the two activities and the game is under one greater picture (i.e., activities earlier in the sequence are designed as clues for activities later in the sequence), the continuity in teaching is enhanced for the core idea "Atom".[39] Second, the Activity is compatible for both in-person and remote settings. Third, in addition to enhancing students' understanding of scientific concepts, this work also aims to promote students' data interpretation ability (e.g., building mathematical models, drawing conclusions based on observed data, etc.).

The activities and the accompanying Web site have been continuously improved since 2019, based on the results. The development and improvement of the learning resource are demand-driven and evidence-based. A description of the implementation and improvements of the activities is available in the Supporting Information (Table S2 and page S8). The following section describes implications for teaching and implementing the activities.

5. FUTURE WORK

Inquiry-learning activities, a subset of the "active learning activities" category, can promote learning during the knowledge construction process assuming high fidelity of implementation.[10,13] Recent studies find that retrieval practice plays a role not only as a measurement instrument but also as an effective learning tool that enhance knowledge retention during the knowledge reconstruction process.[12,17] Thus, retrieval practice is an important complement to the activities in improving the likelihood that students will effectively learn and retain the specific content targeted by the pedagogical tools. Students should engage in such practices that they develop a robust and sustained understanding of atomic orbitals and related concepts. For instance, students should practice sketching atomic orbitals and their RDFs without looking at any notes or the Web site. We recommend following up the activities with extensive formative assessment[40] that could include clicker questions used in a think-pair-share format[41] or exit slip questions.[42] These formative assessments will be most helpful if students refrain from accessing their notes or looking up the representations in a table with the corresponding orbital designation. As we purposefully integrate more formative assessment into the course, we anticipate that student performance on items targeting representational competence and concepts related to atomic orbitals in the

Table 3. Comparison Among Similar Activities

alternative activity	topic	pedagogical approach	environment for implementation: in-person	environment for implementation: remote	results analysis method
Orbital Battleship[36]	Electron configuration	gamification	yes	no	qualitative
Periodic Universe[37]	Periodic properties	inquiry-based learning	yes	no but possible	qualitative and quantitative (pre- and post- test)
Chunking Strategy for Teaching Electron Configuration[38]	Electron configuration	chunking strategy (a memorizing tool)	yes	no but possible	quantitative (control groups)
Activity 1 and 2, BingOrbital (this work)	Atomic orbital isosurface, electron configuration, periodic properties	inquiry-based learning, gamification	yes	yes	qualitative and quantitative (previous cohort as control group)

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summative assessment will increase. Furthermore, if and when rigorously validated assessments or inventories specifically designed to target students' representational competence in the context of atomic orbitals become available, they should be used in a pre-post fashion to better assess learning gains.

In addition, as inquiry learning specifically promotes acquisition of intuitive and deep conceptual knowledge,[16] the type of knowledge the assessment measures should also match.[18] According to the literature, test items involving "recognize", "recall", and "direct application" do not reveal the depth of knowledge. We recommend including test items involving "explanation" and "prediction (transfer and application)". For example, "Do atomic orbitals of hydrogen atom experience penetration and shielding effect? Explain." "A hydrogen atom is excited from the ground state to $n = 2$ energy state. Estimate the energy and the size of the hydrogen atom in excited state with the help of tool 1." The time spent in answering each test item should also be recorded. Such items and the answering time are anticipated to reflect the quality of gained knowledge.[18] Ultimately, it is the hope that the activities and new technology presented here may help to facilitate designing new activities that integrate a greater degree of creativity and imagination in learning chemistry.[43]

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available at https://pubs.acs.org/doi/10.1021/acs.jchemed.1c01023.

Summary of content coverage of activities on ACCM (Table S1), supplemental activity design models (Figures S1 and S2), description of improvements and implementations (Table S2 and page S8), test items (Table S3), users guide for Orbital Explorer and BingOrbital game, instructions of importing moduels on LMS (PDF)

Activity 1: Atomic Orbital Shapes_2021 (PDF, DOCX)

Activity 1: Atomic Orbital Shapes_2021-key (PDF, DOCX)

Activity 1: Atomic Orbital Shapes_2020 (PDF)

Activity 1: Atomic Orbital Shapes_2019 (PDF)

Activity 2: Periodic Properties and Electron Configurations_2021 (PDF, DOCX)

Activity 2: Periodic Properties and Electron Configurations_2021-key (PDF, DOCX)

Activity 2: Periodic Properties and Electron Configurations_2020 (PDF)

Activity 2: Periodic Properties and Electron Configurations_2019 (PDF)

■ AUTHOR INFORMATION

Corresponding Author

Darrin M. York − *Laboratory for Biomolecular Simulation Research, Institute for Quantitative Biomedicine, and Department of Chemistry and Chemical Biology, Rutgers the State University of New Jersey, New Brunswick, New Jersey 08901-8554, United States;* orcid.org/0000-0002-9193-7055; Email: Darrin.York@rutgers.edu

Authors

Xiao Li − *Faculty of Mathematics and Sciences Education, Beijing Institute of Education, Beijing 100120, China; Laboratory for Biomolecular Simulation Research, Institute for Quantitative Biomedicine, and Department of Chemistry and Chemical Biology, Rutgers the State University of New Jersey, New Brunswick, New Jersey 08901-8554, United States;* orcid.org/0000-0003-2616-9333

Marc Muñiz − *Department of Chemistry and Chemical Biology, Rutgers the State University of New Jersey, Piscataway, New Jersey 08854-8087, United States;* orcid.org/0000-0002-0270-3012

Karlun Chun − *Information Technology Office, School of Arts and Sciences, Rutgers the State University of New Jersey, Piscataway, New Jersey 08901, United States*

Jonathan Tai − *Information Technology Office, School of Arts and Sciences, Rutgers the State University of New Jersey, Piscataway, New Jersey 08901, United States*

Francesca Guerra − *Department of Chemistry and Chemical Biology, Rutgers the State University of New Jersey, Piscataway, New Jersey 08854-8087, United States*

Complete contact information is available at: https://pubs.acs.org/10.1021/acs.jchemed.1c01023

Notes

The authors declare no competing financial interest.

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