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Online Orbital Explorer and *BingOrbital* Game for Inquiry-Based Activities

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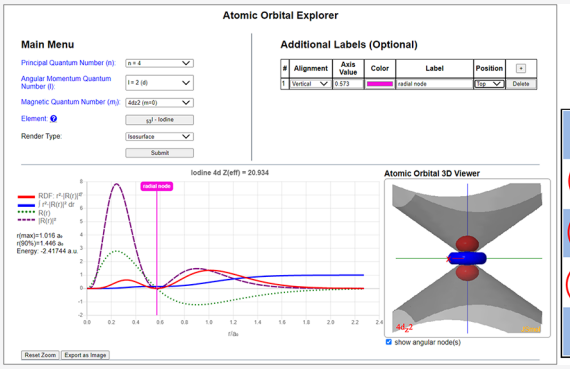

ABSTRACT: We report a new online suite of tools that enables inquiry-based active-learning activities to develop students' representational competence about atomic orbitals. Orbital Explorer is a Web site for the visualization and interactive investigation of atomic orbital properties. Orbital Explorer contains two integrated tools, namely, Atomic Orbital Explorer, which enables one to visualize and interrogate individual atomic orbitals, and Orbital RDF Comparison, which enables one to make a more detailed quantitative comparison of orbital energies and properties of orbital radial distribution functions (RDFs). In addition, we present an original chemistry educational gamification design, BingOrbital, constructed in a format resembling Bingo (American version). The game aims to reinforce the recognition of atomic orbitals based on the RDF and three-dimensional isosurface and has been applied as an engaging retrieval practice tool. A companion set of example activities that use the Orbital Explorer and BingOrbital game have been presented in another article.

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

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1. INTRODUCTION

A detailed understanding of the properties of atomic orbitals and how they relate to periodic trends plays a fundamental role in the understanding of theoretical models for chemical bonding[1] for students of general chemistry. For many students, such an understanding of these often abstract concepts presents a formidable challenge.[2] A pedagogical strategy that has been demonstrated to be successful across multiple domains is to implement an inquiry-based learning (IBL) approach in which students learn knowledge through interrogation and analysis of data in order to solve problems or develop predictive models.[3,4] IBL is a form of active learning that has been demonstrated to be effective in teaching deep, conceptual knowledge,[5] and evidence in the literature suggests that, when meaningfully integrated into undergraduate science, technology, engineering, and mathematics (STEM) classroom environments, IBL can improve student outcomes,[7] narrow achievement gaps,[6,7] and positively impact conceptual understanding and academic skills.[8,9]

This Technical Report presents the Orbital Explorer Web site[10] that contains free[11] online tools for the visualization and interactive investigation of atomic orbital properties to support IBL as well as a complementary engaging game for retrieval practice.[12,13] Building on foundational atomic orbital concepts, such an understanding can ultimately be enhanced by the integration of powerful quantum chemistry/electronic structure theory software tools (e.g., Orca,[14] Multiwfn,[15] ChemCompute,[16] WebMO Basic,[17] etc.) into undergraduate teaching and research. The structure, capabilities, and scope of the online tools and game are described in detail in the sections that follow.

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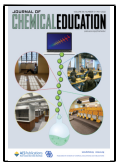

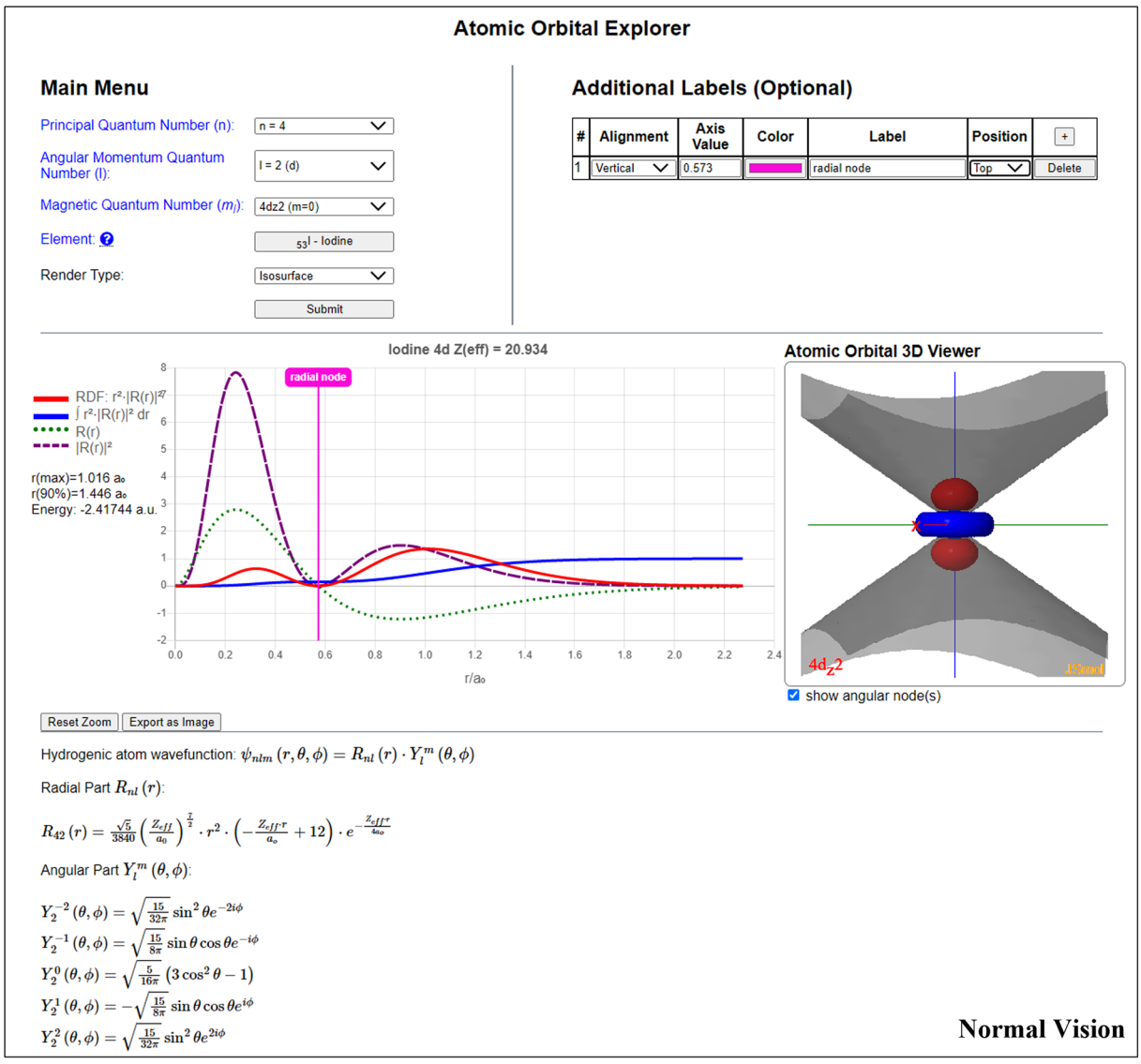

Figure 1. Screen snapshot of Atomic Orbital Explorer[10] (tool 1) webpage displaying a $4d_{z^2}$ orbital with the angular nodes display toggled on and a user-generated vertical line labeled as "radial node" appearing to normal vision.

Table 1. Comparison among Various Visualization Tools for Atomic Orbitals

Name	Tech Requirement	Range of n (principal quantum number)	Types of Available Radial Plots[b]	Z_{eff} Used in RDF?
DIY 3D Models for Hydrogenic Orbitals[28]	3D printer (for making physical models)	$n \leq 4$	None	N/A
Orbital Viewer[29]	Software be installed on a computer prior to class	$n \leq 30$	None	N/A
Hydrogen Atomic Orbital Viewer[a, 30]	Regular browser[a]	$n \leq 16$	RDF	No
Hydrogen Atom Orbital Explorer[31,32]	Regular browser	$n \leq 5$	RDF, R^2, R,	No
Atomic Orbital Explorer[c]	Regular browser	$n \leq 8$	RDF, RDF integral, R^2, R	Yes

[a]Hydrogen Atomic Orbital Viewer requires a Java-enabled browser for the older version[33] (the only available version during the development of this contribution) prior to the latest 2021 release.[30] [b]Radial plots: plots related to the radial component (R) of the atomic orbital wave function (see expression 1). [c]Atomic Orbital Explorer (tool 1) is compared in this table. The Orbital RDF Comparison (tool 2) is developed with the same technologies but has a different format from common orbital visualization tools, so it is not listed for comparison in this table.

2. ORBITAL EXPLORER WEBSITE

The Orbital Explorer Web site[10] contains Atomic Orbital Explorer (tool 1) and Orbital RDF Comparison (tool 2), which visualize important properties of atomic orbitals. A detailed guide for using Orbital Explorer is available in the Supporting Information (pages S3–S8). These tools are designed to support inquiry-based learning activities as "virtual labs" for data collection in the *investigation* phase of an inquiry

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cycle.[18] Technology advancements in recent decades bring more integrations of computer simulation and web technology into inquiry-based learning,[19−22] and such integrations have been shown to promote IBL.[20,23−25] Technologies advance inquiry learning by means of (1) providing visualization tools as scaffoldings,[26] (2) facilitating inquiry processes through interactive platforms on which learners could explore a phenomenon by manipulating variables,[23,25] and (3) revealing unobservable phenomena by computer simulations.[25] The general innovative features of Orbital Explorer that facilitate learning by smoothing instructional logistics, promoting inclusiveness, and providing scaffoldings are introduced in the first subsection below. Chemistry-content-related features that promote learning by addressing learning difficulties are introduced in the following subsections.

2.1. General Features Facilitating Learning

Orbital Explorer (Figure 1) has some advantages in the facilitation of instruction and learning, compared with several other existing tools that visualize atomic orbitals (Table 1). First, technology-wise, all components of Orbital Explorer are implemented in HTML5, lowering the technology requirement for accessing the tools to a functioning browser. Unlike some other tools, no additional software or extensions (e.g., Java) need to be installed. Specifically, radial distribution function (RDF) plots are generated by Python in conjunction with JavaScript, and orbital isosurfaces are generated with JSmol.[27] The accessibility and user-friendliness are greatly enhanced for the web-based learning tools, as there is no strict limitation on the type of electronic device(s) the students use. Most computers and tablets with a mainstream Web browser installed should work. This feature significantly reduces time spent troubleshooting technology-related problems, thus freeing up more time to be spent facilitating the actual activity.

Second, the graphics on the Web site are designed to be barrier-free for color-vision-impaired users.[34] Descriptions of the design principle and a view of tool 1 as it may appear to an individual with deuteranopia (red-green color vision impairment)[34] can be found in the Supporting Information (page S2).

Third, Orbital Explorer is designed to provide an interactive visualization interface to promote students' active participation in learning. "Active learning" refers to a collection of instructional modes that improve student learning outcomes in undergraduate STEM learning environments[6] and is often grounded in constructivist theory.[35] In the context of online learning, it is argued that a Web site that effectively aids learning should not simply provide content but should meaningfully engage students in the learning process (i.e., contain interactive elements that require the use of higher-order thinking skills).[36] The concepts of atomic orbitals reside in the sub-microscopic scale in both the spatial and temporal dimensions and, thus, require the learner to engage in abstract thought or "imagining". Imagining, though beneficial to learning in some circumstances, can have an adverse effect on learning when learners have insufficient prerequisite knowledge.[37] First-year undergraduate students are beginner (novice) learners in the context of atomic orbitals, so a visual representation constitutes an important pedagogical scaffold for them. Research finds multiple-view presentations are more effective than static key views (e.g., anterior, posterior, etc.) only when students can directly control and manipulate the views.[38] To this end, Orbital Explorer provides user-controlled interactive views.

2.2. Radial Distribution Plots with Predictive Value

Orbital Explorer models the radial wave function of atomic orbitals using hydrogen-like wave functions (expression 1) with element- and orbital-dependent effective nuclear charge (Z_{eff}) derived from the optimized orbital exponents of Slater-type orbitals in self-consistent field (SCF) calculations.[39,40] In expression 1

$$R_{n,l}(r) = \sqrt{\frac{(n-l-1)!}{2n(n+l)!}} \cdot \left(\frac{2Z_{eff}}{n}\right)^{l+3/2} \cdot r^{l} \cdot e^{-r\cdot Z_{eff}/n} \cdot L_{n-l-1}^{2l+1}\left(\frac{2r\cdot Z_{eff}}{n}\right) \quad (1)$$

R is the radial wave function, r is the distance from the nucleus, n is the principal quantum number, l is the angular quantum number, Z_{eff} is the effective nuclear charge, and L is the generalized Laguerre polynomial.

The major advantage of using Z_{eff} in hydrogenic wave functions is the more realistic extent of wave function afforded (i.e., appropriate contraction of the orbital for higher Z_{eff}). When $Z = 1$ is used (which is the case for most other atomic orbital visualization tools (Table 1)) for non-hydrogen atoms, the resulting radial distribution function (RDF) is much too diffuse to make physical sense. For example, it is not physically meaningful if one attempts to use the size of a hydrogen 2p orbital ($Z = 1$) to model the behavior of the same orbital in a period 2 element. As the gray line in Figure 2 shows, a 2p orbital with $Z = 1$ has an $r_{95\%}$ (radius enclosing 95% electron density) of 9.15 a_0, which is much larger than the size of any period 2 atom. The van der Waals radius of carbon is 3.2 a_0 (1.70 Å), and that of oxygen is 2.87a_0 (1.52 Å).[41,42] As a comparison, when Z_{eff} for carbon or oxygen 2p orbitals ($Z_{eff} > 1$) is used, the RDF becomes more contracted and comparable to the corresponding atom's size (Figure 2). The extent of Z_{eff}-based RDFs also properly reflects periodic trends. For example, as Figure 2 indicates, the oxygen 2p orbital is more contracted

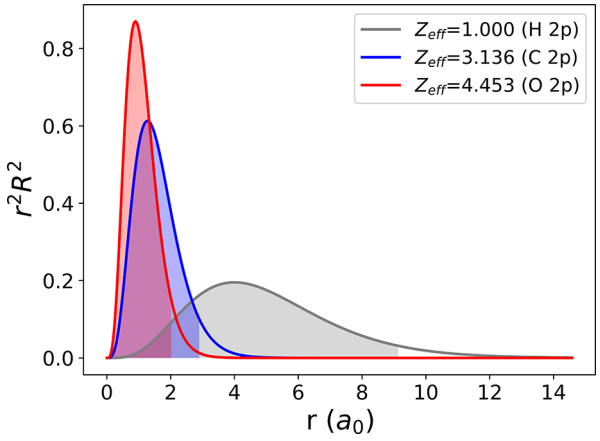

Figure 2. RDF plots of hydrogenic 2p orbitals with the effective nuclear charge (Z_{eff}) of 1 (Z of hydrogen), 3.136 (Z_{eff} of carbon 2p orbital), and 4.453 (Z_{eff} of oxygen 2p orbital) in gray, blue, and red, respectively. The area containing 95% electron density under each RDF is shaded by the same color as the line. The radius enclosing 95% electron density is 9.15 a_0, 2.92 a_0, and 2.04 a_0 for H, C, and O 2p RDF, respectively. As a reference, the van der Waals radius for carbon is 3.2 a_0 (1.70 Å), and that of oxygen is 2.87 a_0 (1.52 Å).[41] The use of orbital-dependent Z_{eff}[39,40] affords RDFs with spatial spans aligning better with experimental radii of neutral many-electron atoms in their ground states.

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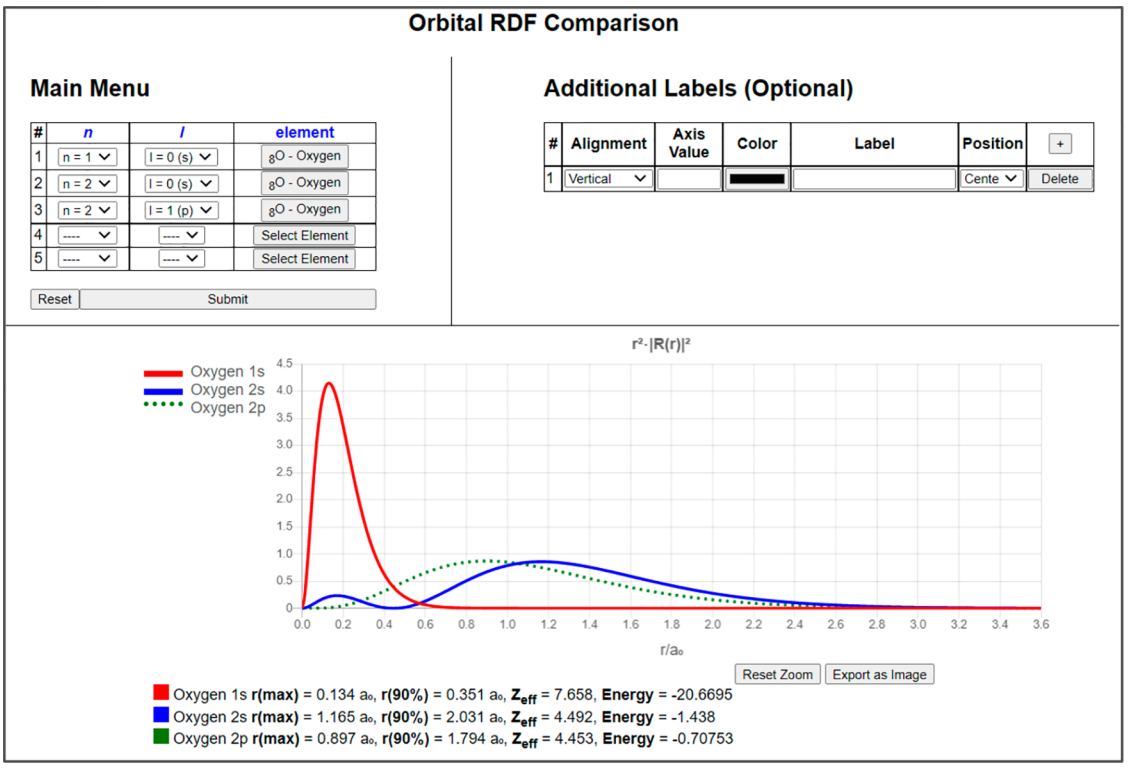

Figure 3. Screen capture of Orbital RDF Comparison[10] (tool 2) displaying overlaid RDFs for oxygen 1s, 2s, and 2p orbitals. R(max) (radius of maximum radial probability), r(90%) (the radius of 90% accumulated radial probability density), Z_{eff} (the effective nuclear charge), and energy computed by the CISD/DGDZVP method of each selected atomic orbital are displayed underneath the RDF plots.

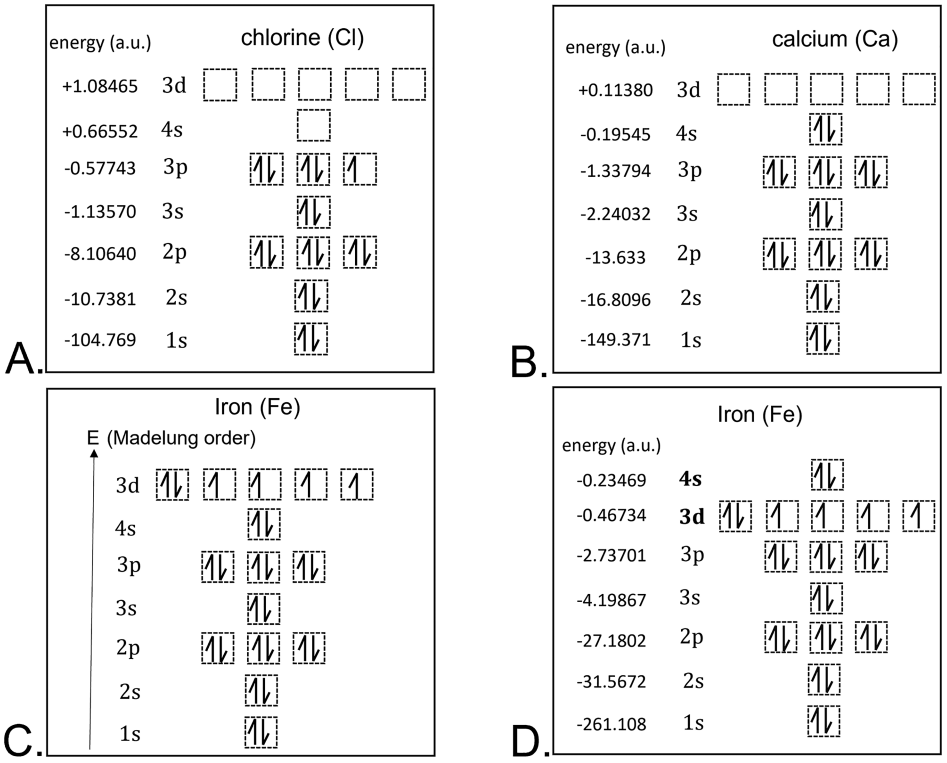

Figure 4. Atomic orbital diagrams of (A) chlorine atom with orbitals ranked by the computed orbital energies, (B) calcium atom with orbitals ranked by the computed orbital energies, (C) iron atom with orbitals ranked by Madelung order, and (D) iron atom with orbitals ranked by the computed orbital energies. The computed energies are calculated with the CISD/DGDZVP method and a Natural Bond orbital (NBO) analysis on Gaussian 16,[47] and the lowest value for a set of α-spin orbitals with the same n and l values are returned upon inquiry (not distinguishing the complexity that sometimes orbitals within the same set will have different energies, e.g., the d-orbitals in Fe and other transition metals).

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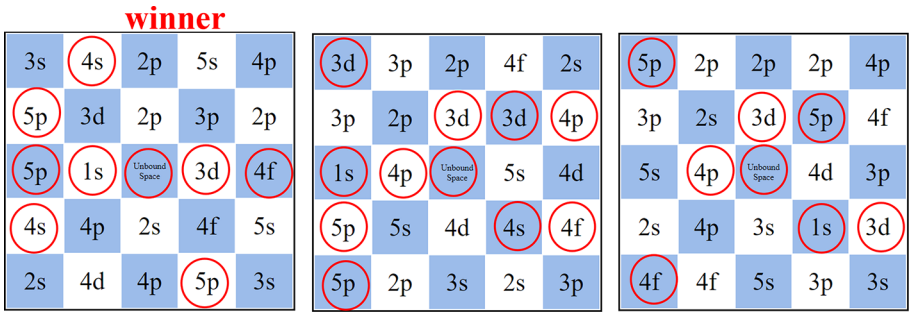

Figure 5. An example of three random BingOrbital cards with circles in a mock game displayed a sequence 1s, 4s, 5p, 3d, 5p, 4p, 3d, 4f orbitals. In the example, the player with the left-most card won. The game card is a 5 × 5 grid with each of the cells filled with an atomic orbital name from 1s to 5p and the center cell filled with "Unbound Space".

than carbon 2p, consistent with the fact that an oxygen atom is smaller than a carbon atom.

Tool 1 presents visual representations and data for one orbital at a time, so the comparison among several orbitals can be performed by opening multiple browser tabs with each tab displaying different orbitals. However, the instructional team deemed it beneficial that the tool be able to display multiple overlapping RDFs. Cognitive load theory also supports the notion that integrating separated information can result in additional cognitive load and create barriers to learning the underlying concepts and skills being targeted by instruction.[43] The Orbital RDF comparison (tool 2) is developed to allow convenient comparison between orbitals. Tool 2 (Figure 3) allows leaners to overlay up to five Z_{eff}-based RDFs. Additionally, computed orbital energies are shown for selected orbitals.

By comparing different orbitals for the same element (Figure 3), students can be guided to discover that (1) orbital energy increases with principal quantum number n when angular momentum quantum number l is held constant; (2) the 2s and 2p orbitals have effective nuclear charges that are clearly smaller than the atomic number as the core electrons shield them; (3) the 2s orbital is lower in energy than the 2p orbital, as it penetrates closer to the nucleus than the 2p orbital.[44]

We note that plugging the effective nuclear charge into hydrogen wave functions (expression 1) approximates atomic orbitals in many-electron atoms for a useful estimation of orbital sizes. This method, however, is not a rigorous quantitative quantum-mechanical model compared to more sophisticated theories, such as Hartree−Fock(HF), Møller−Plesset perturbation (MP2) theory, configuration interaction (CI), and density functional theory (DFT).

2.3. Computed Orbital Energies Aid Addressing Common Misconceptions

Most textbooks[45,46] teach students to follow the Aufbau principle to write electron configurations. While the Aufbau principle with Madelung order (electrons fill in the order of increasing value of $n + l$ with n predominating when two orbitals have the same $n + l$ values, expression 2) works well for main group elements, it fails in predicting the ground-state electron configuration for some transition-metal atoms and all transition-metal cations.

$$1s < 2s < 2p < 3s < 3p < \mathbf{4s} < \mathbf{3d} < 4p < \cdots \quad (2)$$

According to the Madelung order (expression 2), electrons in the 3d orbital should have higher energy than those in the 4s orbital and should be removed before 4s electrons when forming cations for fourth-period transition elements, which contradicts experimental facts. In order to "correct" the Madelung rule, an additional rule stating that "electrons with highest n value should be removed first in the formation of transition metal cations..." is then introduced to students.

There are two types of common misconceptions found arising due to rote recitation of the Madelung rule. Misconception 1, "Madelung order (expression 2) represents the orbital energy ordering in all circumstances".[48] A previous article[48] urges that universities teach students expression 2 as the correct energetic order for only the first 20 and group 1 and 2 elements (Figure 4A,B), but expression 3

$$1s < 2s < 2p < 3s < 3p < \mathbf{3d} < \mathbf{4s} < 4p < \cdots \quad (3)$$

as the correct order for the remaining block-d and -p elements. Misconception 2, "energy levels are a 'fixed rigid ladder' irrespective of electronic configuration (e.g., different electron arrangements/excited states, neutral atom vs ions)".[49,50] These misconceptions detract from students' developing a deep understanding of concepts related to an electronic structure.

The orbital energy data provided by Orbital Explorer enable students to address misconceptions and enhance understanding through inquiry-based activities. Activity 2 described in another paper[51] demonstrates an example activity utilizing the numerical output of energies to overcome learning difficulties associated with writing electron configurations for transition-metal cations. In the activity, students are guided to collect orbital energies for transition-metal atoms (e.g., iron $[Ar]3d^64s^2$), rank the orbitals according to their energies (Figure 4D), and then apply the principle of ionizing electrons with higher energy first to get the electron configuration of the cation (e.g., Fe^{2+}, $[Ar]3d^6$). Through the activity, students verify the orbital energy ordering through data analysis and data interpretation instead of memorizing rules at a superficial level (fact ix in ref 49). The team acknowledges that the Madelung rule (expression 2) is still useful in predicting the "filling order" while expression 3 is useful in predicting the "leaving order" of electrons.

The limitation of the Orbital Explorer Web site is that it provides only limited scaffolding for "anomalous" ground-state electron configurations of the transition elements, which involves other complex theories (e.g., J level, etc.)[48,52−54] that are beyond the scope of first-year undergraduate students. The instructional team considers narratives such as "electrons start to fill 4s before 3d orbitals are full due to repulsions in d-shells", "half-filled and fully-filled d-orbital configuration gain extra stability" as helpful explanations for facts related to such topics (e.g., why the Fe ground state is $[Ar]3d^64s^2$ instead of

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[Ar]3d^8). Because of such a limitation, Activity 2 introduced in another article[51] builds activities based on the provided electron configuration of transition metals.

3. BINGORBITAL—CHEMIST'S VERSION OF THE BINGO GAME

BingOrbital is an original chemistry educational gamification design shared by this contribution. The game aims to practice the recognition of atomic orbitals by RDF and isosurface and has been played in the class following an IBL activity about atomic orbitals (Activity 1 in another Activity paper[51] of this journal) as a form of retrieval practice (drawing information from memory rather than relying on existing notes or a textbook).[12,13] The game is also intended to promote engagement and bring fun to the classroom. This game is constructed in a format resembling American version of Bingo, hence the portmanteau "BingOrbital". In the game, players make effort in recognizing a displayed orbital and circle the orbital on a BingOrbital card (Figure 5).

The first player who circles orbitals in a line (a row, a column, or a diagonal line) and calls out "BingOrbital" wins the game (Figure 5). As the game proceeds quickly and in a competitive environment, students engage in timed retrieval practice.[12,13] They are not afforded time to refer to their notes or the Web site during this activity. Therefore, it serves as a rigorous check of how well they have retained content related to atomic orbitals. The instructions of the game can be found in the Supporting Information (page S7).

4. CLASSROOM IMPLEMENTATION AND FEEDBACK

The Orbital Explorer Web site[10] has been integrated with inquiry-based learning (IBL) activities and has been implemented in the Honors General Chemistry I course at Rutgers University since the Fall 2019 academic term. The IBL activities are described in another publication of this journal and contain two sets of activities: Activity 1 and Activity 2, which are implemented in sequence.[51] Activity 1 focuses on atomic orbital quantum numbers, nodal surfaces, sizes, and energies.[51] Activity 2 focuses on writing electron configurations and periodic trends. The activities guide the students to collect data on Orbital Explorer, and from an analysis of these data to make inferences, identify trends, and create mathematical models. The instructional team generally found that the Orbital Explorer Web site improved the logistics associated with the activity implementation in 2019 compared to 2018 when the activities drew upon a third-party Web site named Hydrogen Atomic Viewer.[33] First, the team experienced fewer technical difficulties caused by a Java installation on browsers. Second, the Orbital Explorer tool provides high-quality, unambiguous representations as effective scaffoldings for IBL. For example, one question repeatedly asked by students to the facilitators is "How do I figure out the number of nodal surfaces associated with this orbital?". As the previous simulation Web site does not allow for the display of nodal surfaces, facilitators spent valuable instructional time answering the question by sketching orbital isosurfaces and providing verbal explanations (with gestures). In the revised version of Orbital Explorer, angular nodal planes can be visualized as transparent gray surfaces by checking the "show angular node(s)" checkbox. In addition, Orbital Explorer serves as a one-stop hub for all types of data (plots of mathematical expressions, three-dimensional surfaces, numerical outputs, etc.) required for the inquiry-oriented activities, so students do not need to collect data across several platforms.

In 2020, during the Covid-19 pandemic, the Web-based tools were found to be highly compatible with remote instruction. The Web site has undergone iterative updates since 2019, based on users' feedback, and the current version is a product of the team's effort in meeting instructors' and students' needs. The usage of the Web site is not limited to the published activities[51] but also enables one to create new learning activities aimed to enhance students' understanding of atomic orbitals and related concepts.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available at https://pubs.acs.org/doi/10.1021/acs.jchemed.1c01277.

Deuteranopia view of Atomic Orbital Explore, users guide for Orbital Explorer and BinOrbital game, sample Gaussian input and output files (PDF)

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Notes

The authors declare no competing financial interest.

Atomic Orbital Explorer Web site: elearning.rutgers.edu/orbitalexplorer.

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