

## SIMULAÇÃO INTERATIVA BASEADA EM INTELIGÊNCIA ARTIFICIAL PARA MODELOS ATÔMICOS: ESTUDO PILOTO

### AI-BASED INTERACTIVE SIMULATION FOR ATOMIC MODELS: PILOT STUDY

### ATOM MODELLERİ İÇİN YAPAY ZEKA TABANLI ETKİLEŞİMLİ SIMÜLASYON: PİLOT ÇALIŞMA

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## RESUMO

**Introdução:** Os modelos atômicos são ensinados de forma abstrata e mecânica, o que limita a compreensão conceitual e as habilidades de raciocínio dos alunos. Este estudo aborda esses desafios por meio de uma simulação interativa baseada em IA que integra o desenvolvimento histórico dos modelos atômicos em uma estrutura tecnológica e pedagógica por meio de diálogos científicos, promovendo a investigação, a participação e a aprendizagem significativa no ensino de química. **Objetivo:** Este estudo tem como objetivo avaliar a eficácia da simulação baseada em IA no desenvolvimento da compreensão conceitual, participação e habilidades de raciocínio científico dos alunos do ensino médio em relação aos modelos atômicos. **Métodos:** O estudo utilizou o método de pesquisa de design e desenvolvimento. A simulação foi criada na plataforma Replit usando a abordagem de diálogo científico suportada pelo GPT-4.0. Cinquenta alunos do 9º ano participaram voluntariamente do estudo. Os dados foram coletados por meio de perguntas abertas e analisados usando escalas de usabilidade, experiência do usuário e carga cognitiva. **Resultados e Discussão:** Os alunos classificaram a simulação como tendo alta usabilidade ( $M=4,07$ ), boa experiência do usuário ( $M=3,76$ ) e baixa carga cognitiva ( $M=2,36$ ). Os comentários qualitativos destacaram que os diálogos científicos eram agradáveis e fáceis de usar. Os resultados mostram que a simulação aumentou efetivamente a compreensão e a participação dos alunos na aprendizagem dos modelos atômicos. O estudo é consistente com trabalhos anteriores que enfatizam o papel das simulações digitais no desenvolvimento da aprendizagem conceitual. O feedback apoiado por IA e os diálogos interativos promoveram a motivação e o raciocínio científico. **Conclusões:** A simulação aumenta a motivação dos alunos e a compreensão conceitual ao integrar elementos históricos, pedagógicos e tecnológicos. Ela apoia a aprendizagem significativa e pode ser expandida com aplicações mais amplas em estudos futuros.

**Palavras-chave:** Educação química, aprendizagem baseada em cenários, tecnologia educacional, compreensão conceitual

## ABSTRACT

**Background:** Atomic models are typically taught using abstract and rote methods, which limit students' conceptual understanding and reasoning skills. This study addresses these challenges through an AI-based interactive simulation that integrates the historical development of atomic models within a technological and

pedagogical framework via scientific dialogues, promoting inquiry, participation, and meaningful learning in chemistry education. **Aims:** This study aims to evaluate the effectiveness of AI-based simulation in developing high school students' conceptual understanding, participation, and scientific reasoning skills regarding atomic models. **Methods:** The study utilized the design and development research method. The simulation was created on the Replit platform using a scientific dialogue approach supported by GPT-4.0. Fifty 9th-grade students volunteered for the study. Data were collected through open-ended questions and analyzed quantitatively and qualitatively using usability, user experience, and cognitive load scales. **Results:** Students rated the simulation as having high usability ( $M=4.07$ ), good user experience ( $M=3.76$ ), and low cognitive load ( $M=2.36$ ). Qualitative feedback emphasized that the scientific dialogues were enjoyable and easy to use. Findings showed increased participation, improved conceptual understanding, and positive learning experiences. **Discussion:** Results suggest that the simulation effectively increased students' understanding and engagement in learning atomic models. Findings are consistent with previous studies highlighting the role of digital simulations in enhancing conceptual learning. AI-supported feedback and interactive dialogues encouraged motivation and scientific reasoning. **Conclusions:** Simulation increases student motivation and conceptual understanding by integrating historical, pedagogical, and technological elements. It supports meaningful learning and can be expanded with broader applications in future studies.

**Keywords:** *Chemistry education, scenario-based learning, educational technology, conceptual understanding*

## ÖZET

**Arka plan:** Atom modelleri genellikle soyut ve ezberci yöntemlerle öğretilir, bu da öğrencilerin kavramsal anlayış ve bilimsel akıl yürütme becerilerini sınırlar. Bu çalışma, bilimsel diyaloglar yoluyla atom modellerinin tarihsel gelişimini teknolojik ve pedagojik bir çerçeveye entegre eden, kimya eğitiminde sorgulama, katılım ve anlamlı öğrenmeyi teşvik eden yapay zekâ tabanlı etkileşimli bir simülasyon aracılığıyla bu zorlukları ele almaktadır. **Amaçlar:** Bu çalışma, lise öğrencilerinin atom modelleriyle ilgili kavramsal anlayış, katılım ve bilimsel muhakeme becerilerini geliştirmede yapay zekâ tabanlı simülasyonun etkinliğini değerlendirmeyi amaçlamaktadır. **Yöntemler:** Çalışmada tasarım ve geliştirme araştırma yöntemi kullanılmıştır. Simülasyon, GPT-4.0 tarafından desteklenen bilimsel diyalog yaklaşımı kullanılarak Replit platformunda oluşturulmuştur. Çalışmaya toplam 50 9. sınıf öğrencisi gönüllü olarak katılmıştır. Veriler açık uçlu sorularla toplanmış ve kullanılabilirlik, kullanıcı deneyimi ve bilişsel yük ölçekleri kullanılarak nicel ve nitel olarak analiz edilmiştir. **Sonuçlar:** Öğrenciler simülasyonu yüksek kullanılabilirlik ( $M=4,07$ ), iyi kullanıcı deneyimi ( $M=3,76$ ) ve düşük bilişsel yük ( $M=2,36$ ) olarak değerlendirmiştir. Niteliksel geri bildirimler, bilimsel diyalogların eğlenceli ve kullanımı kolay olduğunu vurguladı. Bulgular, katılımın arttığını, kavramsal anlayışın geliştiğini ve olumlu öğrenme deneyimleri yaşandığını gösterdi. **Tartışma:** Sonuçlar, simülasyonun öğrencilerin atom modellerini öğrenme konusundaki anlayışlarını ve katılımlarını etkili bir şekilde artırdığını göstermektedir. Bulgular, kavramsal öğrenmeyi geliştirmede dijital simülasyonların rolünü vurgulayan önceki çalışmalarla tutarlıdır. AI destekli geri bildirimler ve etkileşimli diyaloglar, motivasyonu ve bilimsel akıl yürütmeyi teşvik ettiği görülmüştür. **Sonuçlar:** Simülasyon, tarihsel, pedagojik ve teknolojik unsurları entegre ederek öğrencilerin motivasyonunu ve kavramsal anlayışını artırmaktadır. Anlamlı öğrenmeyi desteklemekte ve gelecekteki çalışmalarda daha geniş uygulamalarla genişletilebilir.

**Anahtar Kelimeler:** *Kimya eğitimi, senaryo temelli öğrenme, eğitim teknolojisi, kavramsal anlama*

## 1. INTRODUCTION:

The atom is one of the most important ideas in science, and students need to comprehend it correctly for many fields, including chemistry, physics, and biology. Atomic models are commonly taught in an abstract, rote way in high school chemistry classes, which makes it hard for students to really understand the concepts and leads to many misconceptions (Malkawi *et al.*, 2018; Zarkadis, Stamovlasis & Papageorgiou, 2020; Kaya, 2023). Scientific models connect theories to the real world, making abstract ideas more concrete. However, if this process isn't adequately organized, students' understanding of

concepts stays limited (Justi & Gilbert, 2000; Mansoor & Rodríguez, 2001; Niaz *et al.*, 2002).

The lack of attention to historical and scientific backgrounds, especially in atomic model teaching, is regarded as a major deficiency (Weisi & Zamani, 2015; Cardoso *et al.*, 2020). Currently, interactive computer-based simulations allow students to explore abstract ideas, compare different models, and simulate scientific reasoning procedures (Fabrigas & Paglinawan, 2024; Kefalis, Skordoulis & Drigas, 2025). In particular, PhET Interactive Simulations have been known to promote students' modeling aptitudes and critical comparisons (Wieman, Adams & Perkins, 2008; Moore *et al.*, 2014; Haryadi & Pujiastuti, 2020).

Furthermore, recent discussions regarding the digital transformation of chemistry education emphasize the necessity of technology-supported, sustainable, and pedagogically consistent learning environments (Köfter, Altundağ & Yücel, 2025). In line with this, recent applications of artificial intelligence as well as machine learning in teaching chemistry have great potential to renovate learning environments by providing benefits including, but not limited to, personalized learning, real-time feedback, as well as dynamic content development (Iyamuremye *et al.*, 2024; Maity & Deroy, 2024; Wang *et al.*, 2024; Erümit & Sarıalioğlu, 2025). This research work aims to help students learn and understand atom models through an interrogative approach, drawing on historical and scientific backgrounds. The study seeks to link scientific teaching principles from higher education with learning psychology to help students build concepts (Nadelson *et al.*, 2018; Valeeva *et al.*, 2023). The AI-supported learning environment developed in this direction is designed to holistically support students' conceptual comparison, critical thinking, and historical connectivity skills. The conceptual test and personalized feedback mechanism at the end of the application support the measurement and evaluation process, thereby deepening learning.

This study aims to investigate the integration of AI-supported interactive simulation into the teaching of atomic models, grounded in a historical context. The following questions guide the research:

- How can an AI-supported interactive simulation centered on historical context be adapted to the teaching of atomic models?
- How does such a simulation affect students' conceptual understanding of atomic models?
- How do students rate the usability and level of interaction of the simulation?
- What are the student evaluations regarding the simulation's contribution to the learning process?

The initial design of this study was presented orally at the ICETOL Conference held in Cunda, Ayvalık, on August 26–29, 2025. Based on feedback received at the conference, the simulation was restructured, and the prototype was then tested in a pilot application with high school students.

## 2. MATERIALS AND METHODS:

The methodology of this study was designed to systematically develop, implement,

and evaluate an artificial intelligence-based simulation to help students better understand atomic models. The following sections detail the participants, the study design, the development process, and the data collection procedures.

### 2.1. Participants

The study was conducted with 50 9th-grade students enrolled in public high schools in Ankara, Turkey, during the 2024–2025 academic year. Participation in the study was voluntary, and parental consent was obtained prior to the implementation.

The participants had not yet received formal instruction on atomic theories at the time of the study. The simulation was implemented immediately before the curriculum unit on atomic models to support students' initial conceptual engagement with the topic.

Only students with access to a digital device and the basic skills required to interact with a web-based simulation environment were included. Students who had previously studied atomic theory or did not complete the simulation were excluded from the study. To protect participant privacy, all data were collected anonymously, and no personally identifiable information was recorded.

### 2.2. Study Design

This paper is structured within the Design and Development Research framework (Richey & Klein, 2014). In this study, an artificial intelligence-based simulation environment was designed and developed to support the teaching of atomic models in a historical and interactive context, and its effectiveness was evaluated by using it to high school students.

### 2.3. Development Process and Implementation

The development of the simulation followed a structured instructional design sequence consistent with widely accepted frameworks for multimedia learning environments, particularly the ADDIE model (Analysis, Design, Development, Implementation, Evaluation) (Göçer, Mustafaoğlu, & Alkan, 2026). The design process proceeded through the phases below:

1. Needs and Context Analysis: An examination of high school students' conceptual learning challenges related to atomic models was conducted, informed by existing literature; a concept map was developed based on the Turkish Ministry of National Education's 9th-grade chemistry curriculum (Ministry of National Education [MoNE], 2024).

2. Scenario Development: Original conversations were produced between six scientists from the curriculum (Dalton, Thomson, Rutherford, Bohr, Chadwick, and Heisenberg) while keeping in mind historical authenticity, humorous moments, and curriculum objectives.

3. Digitization and AI Integration: The scenario was turned into an interactive app on the Replit platform. The scientist figure used GPT-4.0-based AI to answer the students' questions.

4. Interface Design: A web interface was created that is easy to use and understand.

5. Assessment Module: At the end of the simulation, there was a test with 10 multiple-choice questions. For each question and the overall assessment, the scientist character provided tailored feedback using artificial intelligence.

### 2.3.1. Needs and Context Analysis

The needs and context study examined the 9th-grade chemistry curriculum issued by the Ministry of National Education of the Republic of Turkey. It identified essential concepts derived from this initiative (MoNE, 2024). The identified topics include aspects of scientific discourse, such as atomic structure, the historical development of atomic models, the experimental data validating these models, and the differing perspectives among scientists. A concept map appropriate for the students' level of conceptual development was developed (Figure 1).

The developed concept map served as the foundation for organizing the simulation content, crafting dialogue scenarios, and establishing evaluation criteria. This analytical procedure was deemed a crucial preparatory step for maintaining pedagogical integrity and creating innovative digital teaching materials aligned with the curriculum.

### 2.3.2. Scenario and Dialogue Development

The basic framework of this simulation is a dialogue among six major scientists (Dalton, Thomson, Rutherford, Bohr, Chadwick, and Heisenberg) who contributed to the modeling of atoms in the past centuries. This scenario is designed to maintain scientific accuracy and educational effectiveness. Jokes, references, and scientific explanations have been evenly incorporated into these dialogues to interest students, provide them with useful context for concepts, and raise their awareness of scientific thinking processes.

The excerpt below is an example of the distinct

writing style as well as scientific debate structure for the characters in the simulation:

- Heisenberg: “Are you still sure where the electron is? I’m not. My uncertainty principle says you can’t know both its location and its speed at the same time.”
- Bohr: “Your ideas have disrupted my orbits. But I admit, the orbital concept is much more accurate.”
- Thomson: “If I hadn’t discovered the electron, none of you would be here. It all started with my plum pudding model!”
- Rutherford: “You talk a good game, Thomson, but I shattered your cake! I found the nucleus with my gold foil experiment.”
- Bohr: “You both did great work, but I brought order to that nucleus. I arranged the electrons into energy levels!”
- Heisenberg: “Did you say order, Bohr? Electrons don’t like discipline. In my world, they’re all a bit lazy and uncertain.”
- Dalton: “You’ve messed up the atom! In my time, everything was simple, clear, and measurable.”
- Chadwick: “Gentlemen, please... Silence. Neutrons don’t talk, but they get the job done.”

In such statements, scientists both argue for their own models and take a critical approach to each other's contributions, thereby revealing the nature of scientific progress. The dialogue framework incorporates features such as intellectual conflict, contrast, and historical context.

These types of discussions enable students to view scientific models not merely as units of knowledge to be memorized, but as systems of ideas that change and evolve scientifically over time and connect with other ideas. In this way, students develop critical thinking, questioning, and conceptual connection skills as they construct scientific models.

### 2.3.3. Technical Implementation and Evaluation Process of the Simulation

The scripted dialogue scenario was transformed into an interactive simulation environment through an AI-powered development process on the Replit platform. This web-based digital learning environment, called “AtomVerse,” combines historically accurate text-based scenarios with character representations, user interactions, and AI-based feedback (Figure 2).

The application is based on system commands modeled using the OpenAI GPT-4.0 model. These system commands have a multi-

layered structure that defines each scientist's style, scientific approach, and interaction method. A total of 11 different GPT-4.0 commands are used in the application, and these commands are organized into three major categories:

1. **Generating Answers to Students' Questions:** Ensures that scientist characters provide contextually and scientifically consistent answers to questions asked by students during discussions.
2. **Test Feedback System:** At the end of the simulation, a 10-question multiple-choice test is presented, and for each question, the relevant scientist character provides explanatory and educational feedback.
3. **Performance Assessment:** The students' overall success, strengths, and areas for improvement are summarized by the analysis module and converted into a personalized final report.

This structure enables students to take on the role of an interactive and curious user who actively participates in their own learning process, rather than merely being an observer (Figure 3). While observing dialogues between scientists, students could ask questions about concepts they want to learn about, and these questions are answered in a scientific manner.

The Graphical User Interface (GUI) was developed on React 18, TypeScript, and Tailwind CSS technologies. During the design process, user experience was prioritized, resulting in a simple, historically aesthetic, and mobile-friendly interface supported by text bubbles, character icons, information cards, and control buttons. Replit's web infrastructure enables this application's online accessibility.

The test at the end of the simulation assesses students' conceptual understanding and guides this process using GPT-4.0-powered explanatory feedback (Figure 4).

Finally, after the test is completed, the system performs data analysis of student performance and generates a personalized final assessment containing a summary of students' achievements and tips for improvement (Figure 5).

Students accessed the application via a

web-based interface and participated in the scientists' interactive discussions. In this way, AtomVerse blends historical, pedagogical, and technological features to offer students an innovative teaching solution that integrates artificial intelligence into chemistry education.

#### **2.4. Data Collection**

A mixed-methods approach was employed to collect data after students engaged in the AtomVerse simulation. The application lasted approximately 20 minutes in total, during which time students accessed the simulation individually in the computer lab. Finally, after completing the simulation, students were asked to complete the AtomVerse Student Experience Survey, which aimed to measure usability, user experience, and cognitive load. The survey included a mixed-methods design comprising five open-ended questions and eleven Likert items, using the UMUX-Lite, UEQ-S, and Cognitive Load Rating Scale tools.

#### **2.5. Data Analysis**

Data collected from the AtomVerse Student Experience Survey was analyzed using both quantitative and qualitative approaches. Quantitative data was processed using IBM SPSS Statistics 26 software to calculate descriptive statistics such as the mean and standard deviation for each dimension of the scale. The internal consistency of the instrument was tested using Cronbach's alpha coefficient, and the normality of the data distribution was checked using skewness and kurtosis values. Repeated measures ANOVA analysis was also used to investigate possible differences between usability, user experience, and cognitive load scales. Qualitative data collected from the five open-ended questions were analyzed using thematic content analysis. Responses were coded inductively to identify recurring themes related to students' learning experiences, perceptions, and suggestions. All analyses were conducted systematically to ensure the validity and reliability of the findings. For open-ended questions, data analysis used thematic content analysis to examine respondents' answers.

### **3. RESULTS AND DISCUSSION:**

#### **3.1. Results**

The results of the Student Experience Survey are presented using both quantitative and qualitative criteria. The results reveal how the

simulation was evaluated in terms of usability, user experience, and cognitive load; they also reflect students' overall perceptions and suggestions thematically.

### 3.1.1. Quantitative Findings

The survey data were collected from 50 9th-grade students. The scale is a 5-point Likert-type scale and consists of 11 items. Three sub-dimensions were evaluated. Representative sample items from each sub-dimension are provided below:

- Usability (UMUX-Lite): “The application meets my needs.” / “It was easy to use.”
- User Experience (UEQ-S): “The application was fun.” / “It looked good.” / “It was motivating.”
- Cognitive Load: “The application was mentally exhausting.” (negative item)

According to the analysis results, the reliability coefficient of the scale was found to be Cronbach's  $\alpha=0.73$ ; this value indicates that the scale has an acceptable level of internal consistency.

Repeated Measures ANOVA results revealed a significant difference among dimensions,  $F(2, 98) = 63.48$ ,  $p < .001$ . Students' perceptions of AtomVerse are ranked by average score in Table 1.

These results indicate that students generally evaluated the application as an easy, motivating, and supportive learning environment. In particular, the items “Easy to use” ( $\bar{x} = 4.22$ ) and “I found it generally good” ( $\bar{x} = 4.22$ ) received the highest scores. In contrast, the items “It was creative” ( $\bar{x} = 3.12$ ) and “It was interesting” ( $\bar{x} = 3.46$ ) received relatively lower scores, indicating that the depth of interaction could be increased by diversifying the application's content.

**Table 1.** Dimension-Based Average Results for the AtomVerse Application

Dimension	Mean ( $\bar{x}$ )	Std. Dev.	Comment
Usability	4.07	0.85	The application is user-friendly and easy to find.
User Experience	3.76	0.66	Aesthetic, motivational, and entertainment elements are strong.
Cognitive Load	2.36	1.06	The application was not found to be mentally taxing.

### 3.1.2. Quantitative Findings

A content analysis of the five open-ended questions in the AtomVerse Student Experience Survey was conducted, and codes were created based on the themes. The codes for each question were supported by sample statements taken directly from the students' opinions.

Question 1: “What did you like most about using the AtomVerse application?” Two main codes emerged from this question: Scientific Dialogue and Interaction. The statements belonging to the scientific dialogue code are as follows: “I liked the scientists bantering with each other” (S12), “Scientists talking among themselves” (S24). The statements related to the Interaction code are as follows: “I liked that it answered my questions” (S32), “Being able to ask questions” (S37).

Students particularly liked the dialogues and discussions between scientists. The expressions “asking questions” and “getting answers” were frequently repeated. This shows that students perceived the interactive and humorous learning environment positively.

Question 2: “Was there any point where you struggled while using the application?” According to the content analysis, a single code emerged from this question: Ease of Use. Statements related to the easy-to-use code: “The messages came one after another, so I couldn't understand them easily” (S1), “The application was easy” (S15), “It was very easy and explanatory” (S28).

The vast majority of students stated that they did not experience any difficulties. Although some students noted that the messages passed quickly, the general opinion is that the application

is easy to understand.

Question 3: “How did this application help you learn atomic models?” According to the content analysis of this question, two codes were identified: Retention and Fun Learning. Statements belonging to the Retention code: “It opens your mind and becomes lasting” (S7), “It made it more memorable” (S26), “I understood the topic while Dalton and his friends were discussing it” (S36). Expressions belonging to the Fun Learning code: “It was fun because it was like a game” (S7), “It explains things in a fun way” (S34), “Both fun and educational” (S30).

The majority of students directly used the expression “it was helpful.” The prominence of the “lasting learning” and “fun learning” codes supports the idea that the application functions as a tool that facilitates learning.

Question 4: “What was the difference compared to regular classes?” Two codes emerged from this question: Active Learning and Attractiveness. Statements related to the Active Learning code: “It has an educational artificial intelligence” (S10), “It was different and nice because it was both technological and answered my questions” (S18), “The environment was comfortable because it could be done outside of school” (S36). Expressions related to the attention-grabbing code: “It was nicer because it was in a digital environment” (S41), “It created a nice difference” (S49), “It was both different and made learning easier” (S46).

Students described the application as “more fun,” “more attention-grabbing,” and “better.” These findings show that AtomVerse increases active participation and motivation, unlike traditional lessons.

Question 5: “What changes would you suggest improving the application?” Two codes emerged from the content analysis: Audio Narration and Visual-Auditory Enrichment. Statements related to the audio narration code: “I would like audio to be added” (S5), “Audio could be added, AI could speak in a more human-like way and be a little more argumentative when discussing” (S11), “There could be a read-aloud feature and slower messaging” (S24). Expressions related to the visual-audio enrichment code: “The text could be larger and faster” (S22), “There could be an impressive background” (S28), “The background is overwhelming, it could be changed” (S35).

The most frequently mentioned suggestion was to add a “voice feature” to the application. Some students also suggested adding new

features or diversifying response formats. Overall, students are satisfied with the application, and their suggestions are focused on improvement.

### 3.2. Discussions

The AtomVerse simulation illustrates an original methodology that integrates historical, pedagogical, and technological consistency in the instruction of atomic models. Presenting scientific concepts within a historical timeline and addressing them comparatively supports students’ ability to establish conceptual integrity and develop a consistent mental model of atomic theory.

The representation of scientists using the language specific to their own era exemplifies the adaptation of the scenario-based learning approach (Schank *et al.*, 1994) and the theory of concept development through sociocultural interaction (Vygotsky & Cole, 1978) to a digital learning environment. This structure facilitates the transformation of abstract scientific concepts into concrete experiences, enabling students to construct meaning through active interaction and reflection.

Consistent with previous work in the field (Fabrigas & Paglinawan, 2024; Kefalis, Skordoulis, & Drigas, 2025), digital simulations have been shown to facilitate the understanding of complex and abstract concepts. In this regard, AtomVerse provides a personalized and interactive learning experience for students. Furthermore, an entertaining depiction of scientists helps students become emotionally engaged in the learning process, whereas scientific dialogues in an interactive test module help foster students’ scientific argumentation skills.

Finally, the performance analysis using AI in this simulation helps students know their areas of proficiency as well as those that require improvement, contributing to students’ self-awareness and self-regulation skills. Thus, AtomVerse goes beyond being a mere information-transferring system to offer an interactive learning environment where the student is an active part of their own learning process.

## 4. CONCLUSIONS:

This study creates, implements, and develops AtomVerse, an interactive simulation utilizing artificial intelligence technologies, thereby offering a new solution that provides a coherent combination of historical, pedagogical, and technological consistency in the teaching of atomic models.

Quantitative findings from the implementation process show that students rated AtomVerse as extremely user-friendly (average usability score:  $4.07 \pm 0.85$ ), motivating, and cognitively non-challenging (low cognitive load:  $2.36 \pm 1.06$ ). These results highlight the simulation's accessible and functional structure, enabling smooth navigation without mental exhaustion. Qualitative insights reveal that students particularly value interactive elements such as "scientific dialogues" and "opportunities to ask questions," describing this experience as more engaging, dynamic, and enjoyable compared to traditional lessons. This feedback highlights AtomVerse's role in promoting meaningful learning in both cognitive and sensory dimensions and is consistent with previous research on digital simulations in chemistry education (Fabrigas & Paglinawan, 2024; Kefalis, Skordoulis, & Drigas, 2025).

As detailed in the discussion, AtomVerse goes beyond mere knowledge transfer by providing an interactive environment where students actively construct knowledge. The scientists' dialogues exemplify the adaptation of scenario-based learning (Schank *et al.*, 1994) and Vygotsky's sociocultural interaction theory (Vygotsky & Cole, 1978) to the digital context, transforming abstract, atomic concepts into concrete, reflective experiences. From a technological standpoint, Replit is the platform used to create this simulation, relying on a web-based integrated development environment (IDE) for collaborative coding, real-time preview, and API connectivity to artificial intelligence systems for data analysis, after consideration of other platforms including Glitch, CodeSandbox, Firebase/Vercel, and Cursor, which were eliminated for Replit's ease of accessibility, development speed, multiple-user capabilities, as well as completely web-intuitive deployment capabilities regardless of device types for more sustainable purposes in different contexts of educational applications.

Consequently, AtomVerse distinguishes itself as a singular simulation that seamlessly integrates historical background, comedic

features, and AI-driven personalized feedback, setting it apart from conventional tools such as PhET, ChemCollective, and Labster through its cohesive content delivery approach. While PhET primarily focuses on interactive visualizations, Labster emphasizes virtual laboratory experiments. AtomVerse, on the other hand, offers a narrative-driven, dialogue-based interaction model that contextualizes scientific knowledge within its historical development. It effectively enhances the conceptual understanding of atomic models, increases learning motivation, and develops scientific argumentation skills, demonstrating the transformative potential of AI-focused simulations in chemistry education.

However, limitations remain, particularly regarding the accuracy of GPT-4.0 responses, which depend on the quality of the command. To mitigate this, auditable feedback mechanisms are recommended to enhance system reliability. These mechanisms may include logging responses, automatic fact-checking layers (e.g., cross-verification with reliable databases), human-supervised hybrid models, or user feedback loops; thus, consistency is enhanced through prompt optimization (e.g., using standard prompt structures like ROT), while the pedagogical integrity of educational outputs is preserved. Future work could further strengthen the reliability of AI-based tools by integrating these approaches. In the future, AtomVerse, with its student-centered, interaction-focused, and pedagogically sound structure, promises broader integration into educational ecosystems. Future adaptations may include audio narration, audiovisual enhancements, language options, and applications for various age groups, further increasing its inclusivity and impact.

## 5. DECLARATIONS

### 5.1. Study Limitations

Several limitations should be considered when interpreting the findings of this study. The research adopted a design-and-development methodology; therefore, the findings primarily reflect the pedagogical potential, practicality, and applicability of the AtomVerse simulation rather than its causal effects on students' learning outcomes. Consequently, conclusions regarding instructional effectiveness should be interpreted within the boundaries of exploratory and developmental research.

The study involved a sample of 50 ninth-grade students from public high schools in a single

urban location, using convenience sampling. The small sample size and non-random sampling method limit the applicability of the findings to broader student populations, diverse school types, and varying socio-educational contexts.

Resource and equipment constraints also need to be acknowledged. Effective use of the AtomVerse simulation requires access to digital devices and a stable internet connection, which may not be equally available across all educational settings. In addition, the effectiveness of the AI-supported feedback mechanism depends on prompt design quality and the response-generation characteristics of the GPT-4.0 model, which may influence the consistency, depth, and precision of the feedback provided to students.

This study, which focuses mostly on atomic models, is especially pertinent to high school chemistry classes. As a result, even though the findings hold true for comparable grade levels and learning resources, pedagogical, contextual, and content-specific modifications may be necessary to make them applicable to different academic fields or educational phases.

The study confines its focus to the design of the AtomVerse simulation and its preliminary implementation in the classroom. This study does not consider long-term learning outcomes, knowledge retention, or comparative effectiveness evaluations relative to conventional teaching methods. Subsequent research may mitigate these constraints by utilizing longitudinal designs, involving larger and more diverse populations, and adopting experimental or comparative methodologies.

Notwithstanding these constraints, the study offers significant insights into the pedagogical framework and classroom implementation of AI-enhanced simulations in chemistry teaching, establishing a robust basis for subsequent research.

## 5.2. Acknowledgements

The authors would like to thank the school administrators and chemistry instructors who took part for facilitating the implementation process and providing logistical support during the classroom application. The authors also thank the student participants for their engagement and valuable feedback, which contributed to the practical evaluation of the AtomVerse simulation in an authentic learning environment.

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In accordance with Periódico Tchê Química's ethical guidelines, which prohibit donations from authors with manuscripts under review (even when research funds are available), or in cases of author financial constraints, publication costs were fully absorbed by the journal under our Platinum Open Access policy, with support from Araucária Scientific Association (<https://acaria.org/>). This policy ensures complete independence between the editorial process and any financial aspects, reinforcing our commitment to scientific integrity and equitable knowledge dissemination.

## 5.4. Conflicts of Interest

The authors declare no conflicts of interest and no competing interests.

## 5.5. Data Availability

Raw data are available upon request from the corresponding author ([billurwork@gmail.com](mailto:billurwork@gmail.com)) due to participant confidentiality and ethical restrictions.

## 5.6. Author Contributions

Billur Köfter: Conception and design, data collection, data analysis and interpretation, manuscript writing, final approval.

Fatma Alkan: Conception and design, data analysis and interpretation, critical review, final approval.

Ayşem Seda Yücel: Conception and design, critical review, final approval.

## 5.7. AI and Computational Tools Declaration

Tool: ChatGPT (OpenAI). Purpose: Language refinement, structural editing, and assistance with initial drafting of selected manuscript sections. Extent: Approximately 10% of manuscript preparation. All AI-generated content used during manuscript preparation was reviewed, critically revised, and approved by the authors.

In addition, the AI-based interactive simulation examined in this study (AtomVerse) was developed and implemented on the Replit platform using the GPT-4.0 model as part of the research design. The use of artificial intelligence in the simulation constituted the subject of the study itself.

No artificial intelligence tools were used for data fabrication, statistical analysis, interpretation of results, or scientific decision-making.

## 5.8. Research Integrity Declaration

The authors certify that this research complies with the standards of research integrity, including no data fabrication, no results falsification, no p-hacking or selective reporting, originality, not previously published, and ethical methods.

An earlier version of the study design was presented as an oral presentation at the ICETOL Conference (August 26–29, 2025); however, the present manuscript includes substantial revisions, expanded implementation, pilot data, and extended analysis, and has not been previously published in any journal.

## 5.9. Originality & Plagiarism Statement

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## 6. STUDIES INVOLVING HUMANS AND ANIMALS

### 6.1. Ethics Committee Approval

The Hacettepe University Graduate School

of Educational Sciences Research Ethics Committee approved this study. Ethical approval was granted under application number E-51944218-050-00004774535 on 17 February 2026, following full committee review.

All procedures involving human participants were conducted in accordance with the Declaration of Helsinki. Written informed consent was obtained from parents or legal guardians, and written voluntary participation forms were obtained from all student participants prior to data collection.

### 6.2. Informed Consent

Written informed consent was obtained from parents or legal guardians of all underage participants, and written voluntary participation forms were obtained from all students prior to data collection. Participants were fully informed about the study's purpose, procedures, and scope.

All data were collected anonymously, and no personally identifiable information was recorded. Participants were informed that their involvement was entirely voluntary, that they could withdraw at any time without any consequences, and that participation would have no impact on their academic standing. All collected data were used solely for research purposes and securely stored to ensure confidentiality and privacy.

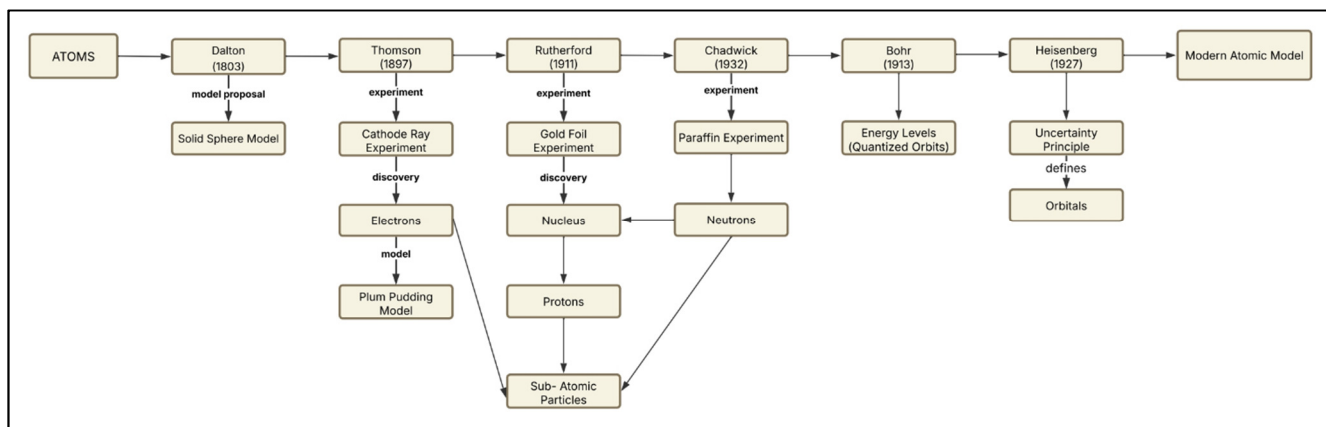
## 7. REFERENCES:

1. Cardoso, P. S. S., Nunes, M. C. S., Silva, G. P. S., Braghittoni, L. S., & Trindade, N. M. (2020). Conceptions of high school students on atomic models, radiation and radioactivity. *Physics Education*, 55(3), 035030.
2. Erümit, A. K., & Sarıalioğlu, R. Ö. (2025). Artificial intelligence in science and chemistry education: A systematic review. *Discover Education*, 4(1), 178.
3. Fabrigas, E. J. A., & Paglinawan, J. L. (2024). Digital simulation exposure and conceptual understanding in chemistry. *International Journal of Research and Innovation in Social Science*, 8(12), 741–747.
4. Göçer, M., Mustafaoğlu, F. M., & Alkan, F. (2026). Use of Web 2.0 Tools in Science Education: Designing Multimedia Learning Environments with the ADDIE Model. In *AI-Powered Educational Games and*

- Simulations* (pp. 117-158). IGI Global Scientific Publishing.
5. Haryadi, R., & Pujiastuti, H. (2020, April). *PhET simulation software-based learning to improve science process skills*. In *Journal of Physics: Conference Series*, 1521(2), 022017. IOP Publishing.
  6. Iyamuremye, A., Niyonzima, F. N., Mukiza, J., Twagilimana, I., Nyirahabimana, P., Nsengimana, T., ... & Nsabayezu, E. (2024). Utilization of artificial intelligence and machine learning in chemistry education: a critical review. *Discover Education*, 3(1), 95.
  7. Justi, R., & Gilbert, J. (2000). History and philosophy of science through models: some challenges in the case of 'the atom'. *International journal of science education*, 22(9), 993-1009.
  8. Kaya, A. (2023). Addressing Student Misconceptions about Atoms and Examining Instructor Strategies for Overcoming Them. *Journal of Pedagogical Research*, 7(4), 251-262.
  9. Kefalis, C., Skordoulis, C., & Drigas, A. (2025). Digital simulations in STEM education: Insights from recent empirical studies, a systematic review. *Encyclopedia*, 5(1), 10.
  10. Köfter, B., Altundağ, C. K., & Yücel, A. S. (2025). A Step Beyond in Industrial Chemistry Education: Digitalization and Sustainability. In *Digital Transformation and Sustainability in Higher Education* (pp. 133-170). IGI Global Scientific Publishing.
  11. Maity, S. & Deroy, A. (2024). Generative AI and its impact on personalized intelligent tutoring systems. *arXiv preprint arXiv:2410.10650*.
  12. Ministry of National Education (MoNE). (2024). *Chemistry curriculum for upper secondary education (Grades 9–12): Türkiye's Century Education Model*. Directorate General of Board of Education.
  13. Malkawi, E. O., Obeidat, S. M., Al-Rawashdeh, N. A., Tit, N., & Obaidat, I. (2018). Misconceptions about atomic models amongst the chemistry students. *International Journal for Innovation Education and Research*, 6(2), 156-263.
  14. Mansoor, N., & Rodríguez, M. A. (2001). Do we have to introduce history and philosophy of science or is it already 'inside' chemistry? *Chemistry Education Research and Practice*, 2(2), 159–164.
  15. Moore, E. B., Chamberlain, J. M., Parson, R., & Perkins, K. K. (2014, July 2). *PhET Interactive Simulations: Transformative Tools for Teaching Chemistry*. *Journal of Chemical Education*, 91(8), 1191–1197.
  16. Nadelson, L. S., Heddy, B. C., Jones, S., Taasoobshirazi, G., & Johnson, M. (2018). Conceptual change in science teaching and learning: Introducing the dynamic model of conceptual change. *International Journal of Educational Psychology*, 7(2), 151–195.
  17. Niaz, M., Aguilera, D., Maza, A., & Liendo, G. (2002). Arguments, contradictions, resistances, and conceptual change in students' understanding of atomic structure. *Science education*, 86(4), 505-525.
  18. Richey, R. C., & Klein, J. D. (2014). *Design and development research: Methods, strategies, and issues*. Routledge.
  19. Schank, R. C., Fano, A., Bell, B., & Jona, M. (1994). The design of goal-based scenarios. *The Journal of the Learning Sciences*, 3(4), 305–345.
  20. Valeeva, R., Biktairova, G., Lesev, V., Mikhailenko, O., Skudareva, G., & Valentovinis, A. (2023). *Exploring the impact of modeling in science education: A systematic review*. *Eurasia Journal of Mathematics, Science and Technology Education*, 19(6), em2284.
  21. Vygotsky, L. S., & Cole, M. (1978). *Mind in society: Development of higher psychological processes*. Harvard University Press.
  22. Zarkadis, N., Stamovlasis, D., & Papageorgiou, G. (2020). Student ideas and misconceptions for the atom: A Latent Class Analysis with covariates. *International Journal of Physics and Chemistry Education*, 12(3), 41-47.
  23. Wang, S., Wang, F., Zhu, Z., Wang, J., Tran, T., & Du, Z. (2024). Artificial intelligence in education: A systematic literature review. *Expert Systems with Applications*, 252, 124167.
  24. Weisi, H., & Zamani, G. (2015). A comparison of the cognitive taxonomy of

educational objectives to the evolution of the atomic theory. *Enjoy Teaching Journal*, 3(3), 1–8.

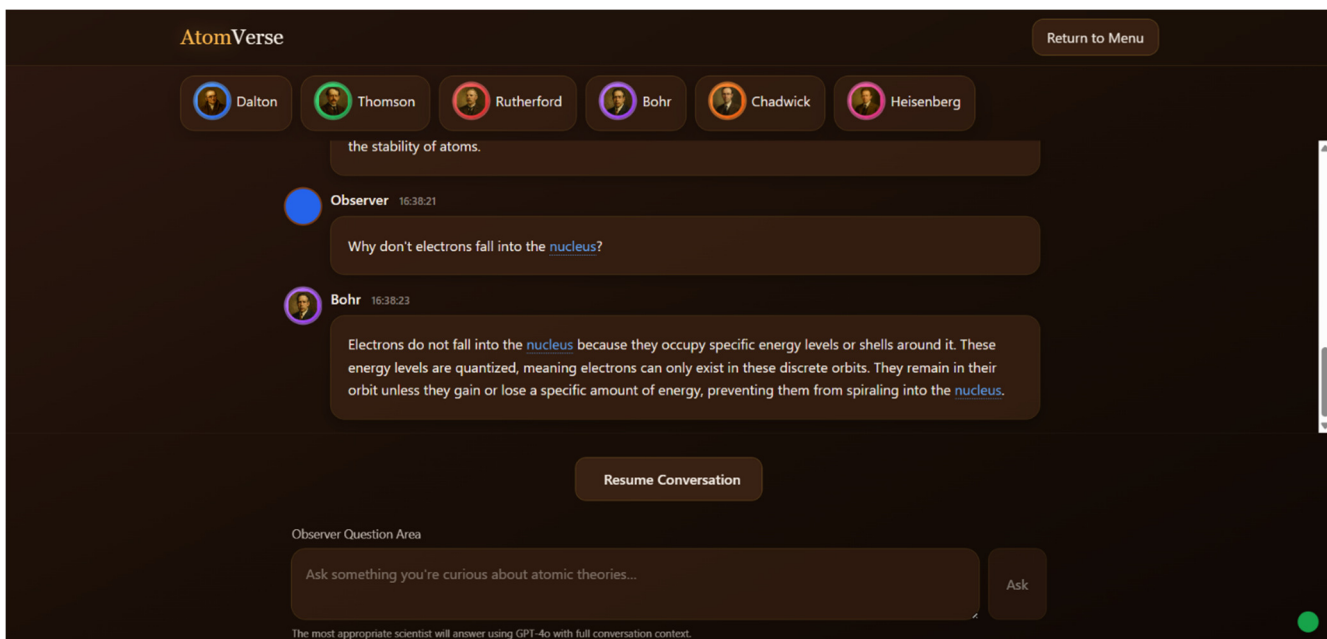
25. Wieman, C. E., Adams, W. K., & Perkins, K. K. (2008, October 31). PhET: Simulations that enhance learning. *Science*, 322(5902), 682–68



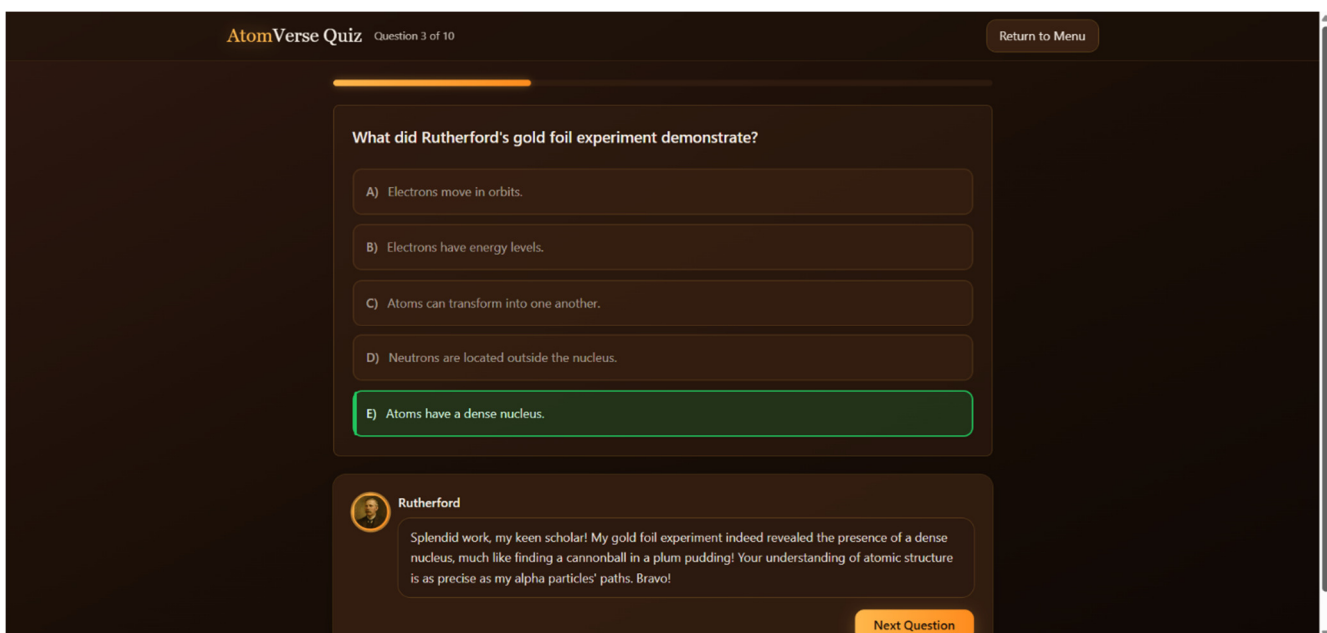
**Figure 1:** Concept map representing the historical development of atomic models, showing the contributions of six key scientists (Dalton, Thomson, Rutherford, Chadwick, Bohr, and Heisenberg) and their experimental and theoretical findings.



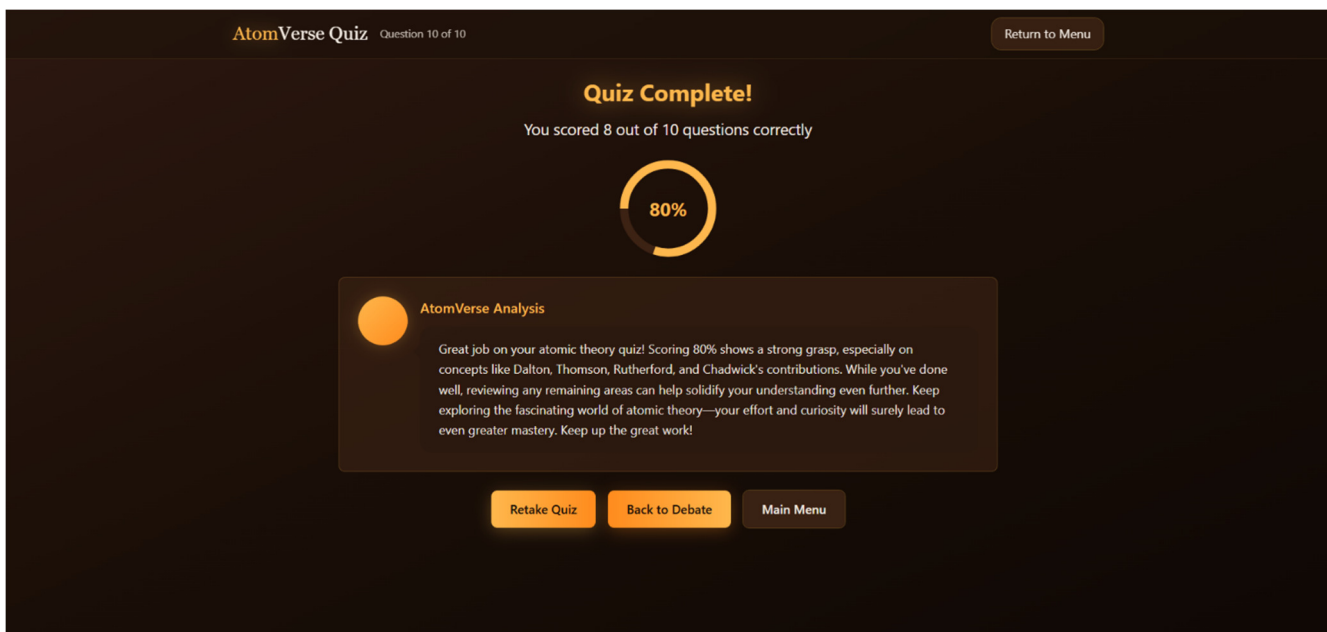
**Figure 2:** The opening screen introduces students to the simulation and provides access to scientists' dialogues. It serves as the main navigation center where users can start their learning session and enter the assessment module.



**Figure 3:** Interactive dialogue screen in the AtomVerse simulation. The student asks a scientist a direct question and receives a response generated by artificial intelligence. This environment enables real-time interaction.



**Figure 4:** An example screen from the AtomVerse test module. The test module enables students to answer conceptual questions and receive automatic feedback, helping assess their understanding after completing the simulation.



**Figure 5:** The evaluation screen summarizes students' overall performance in the test module simulation with artificial intelligence support; it displays students' scores, feedback, and progress in conceptual understanding.