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VISUALIZING CRYSTAL STRUCTURES: ADVANCING DIGITAL LITERACY IN DISTANCE LEARNING

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Abstract

In the increasingly advanced digital era, distance learning has become crucial at all levels of education, especially due to the impact of the COVID-19 pandemic. While distance learning offers flexibility, it also presents challenges in teaching complex subjects such as crystallography, which require visualization for comprehensive understanding. Consequently, it's important to enhance students' digital literacy. The research objective was to explore the role of technology, specifically Diamond software, in visualizing crystal structures to develop students' digital literacy. The research used a descriptive qualitative approach involving students taking Solid-state physics courses within a distance learning system. Data was gathered through digital literacy tests (pre-test and post-test), interviews, and observations of student interactions with Diamond software, which were then analyzed using thematic analysis. This research also emphasizes the differences between independent and guided learning methods. The research results show that Diamond software significantly enhances students' digital literacy, particularly in technological skills, understanding crystallography concepts, and being ethical about data sources and visualization results. These findings indicate that technology-based learning (3D simulation) with guided learning can effectively promote digital literacy and aid students in comprehending specific concepts (crystal structure) in distance learning, particularly in science education.

Keywords: Diamond software, digital literacy, distance learning, visualization of crystal structure

1 INTRODUCTION

Distance learning has evolved rapidly, especially since the COVID-19 pandemic, which compelled educational institutions to quickly adapt to digital technology (Ahmed & Opoku, 2022). This development has driven a transformation in education, not only in teaching methods but also in the competencies required for students to succeed in a digitally integrated learning environment (Bonfield et al., 2020). One of these competencies is digital literacy, which encompasses understanding, accessing, and critically evaluating digital information (Spante et al., 2018). In science education (crystallography), it is crucial because a deep understanding of crystal structures requires conceptual knowledge and visual comprehension.

Before the digital era, learning media for crystal structures primarily consisted of physical models or static images, which had limitations in representing the complexity of crystal structures (Rusnayati et al., 2023). For example, the ball-and-stick models help illustrate atoms and interatomic bonds in simple cubic crystal structures but are limited in presenting variations in the perspective and dynamic of the structures interactively (Elsworth et al., 2017). These limitations become a challenge in distance learning, where non-multimedia tools are not sufficient to help students gain a complete understanding of the crystal structures' complexity (Andreev et al., 2021). Therefore, various digital technology-based visualization media for crystal structures have been developed to facilitate the understanding of complex crystal structures and are widely applied in education and research (Casas & Estop, 2015).

Currently, technology-based visualization has become an effective solution to conventional media limitations, such as 3D visualization in various software, allowing students to rotate, zoom in, and view crystal structures from multiple angles, thus providing an interactive experience (Dalacosta & Pavlatou, 2019; Eriksen et al., 2020). *CrystalExploreri* visualizes and analyzes molecular structures with a focus on Hirshfeld surfaces and vacancy spaces within the crystal (Spackman et al., 2021). *CrystalMaker* enables users to build and manipulate crystal structures with an intuitive interface and simulates the physical properties (Palmer, 2015). *Vesta* visualizes three-dimensional crystal structures and electron density distributions, that help the understanding of atomic interactions in the crystal lattice (Momma & Izumi, 2011). *Diamond* provides detailed graphical representations with high resolution and supports various input and output formats (Khusnani et al., 2022). *Mercury* displays multiple crystal structures simultaneously and allows for direct comparisons (Macrae et al., 2020). In crystal modeling, CIF (Crystallographic Information Framework) data is a standard format for storing and exchanging crystal structure data, facilitating compatibility between software, analysis, and visualization (Bruno et al., 2017). Additionally, web-based simulations, such as *Jmol*, allow users to explore crystal structures directly through their browsers without the need for additional software installation (Dalacosta & Pavlatou, 2019; Hanson, 2010). This is especially beneficial in distance learning, where accessibility and ease of use are crucial factors (Andreev et al., 2021).

As the use of technology in distance learning increases, students' digital literacy becomes essential (Mujtahid et al., 2021; Spante et al., 2018). Digital literacy in science education encompasses not only the technical skills to use software but also the cognitive abilities to understand complex visual information (Caton et al., 2022; Iordache et al., 2017). The use of these visualization tools significantly supports the enhancement of students' digital literacy, helping them grasp complex crystallography concepts and develop their digital technical skills (Kumar et al., 2021; Vodă et al., 2022). Research by Saidin (2015) has demonstrated that interactive visualization tools are more effective than conventional media in enhancing the understanding of abstract materials (Saidin et al., 2015), such as molecular dynamics (Hospital et al., 2015), chemical reactions (Lu & Chen, 2021), and crystal structure (Spackman et al., 2021). In addition, guidance also a crucial role in distance learning, helping students access and utilize technology effectively. The guidance can enhance students' ability to utilize technology, addressing the digital literacy gaps in distance learning (Mishra & Koehler, 2006). Thus, digital literacy serves as a foundation for crystallography education in the digital era.

The research objectives are to fill a gap in the literature regarding the use of 3D visualization technology in distance learning. While many studies have highlighted the effectiveness of computer-based simulations in science visualization, there is still a limited focus on crystallography in distance learning. This research explores the use of Diamond software to aid students in visually understanding crystal structures, to enhance their digital literacy. Additionally, this research emphasizes the importance of digital literacy in technology-based education, particularly in guided distance learning (Mohammadyari & Singh, 2015).

2 METHODOLOGY

This research used a descriptive qualitative approach to explore how crystal visualizing technology can enhance students' digital literacy in distance learning (Bruno et al., 2017). Data were collected through tests, semi-structured interviews, and observations (Sugiyono, 2022). The tests and interviews were conducted coherently to measure digital literacy, while observations were used to assess students' interactions with the Diamond software and their digital ethics during the learning process (Taherdoost, 2021). The research instruments developed based on the digital literacy model proposed by Calveni (2008) were technological, cognitive, and ethical dimensions (Calvani et al., 2008) as presented in Table 1. The instruments were developed into 25 open-ended questions, each scored on a scale of 0 to 5.

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***Table 1**. Digital literacy instruments in technological, cognitive, and ethical dimensions*

No.	Dimensions	Indicators
1	Technological	1A. Operating Diamond software 1B. Processing crystal databases 1C. 3D simulation and visualization 1D. Processing and exporting visual data
2	Cognitive	2A. Identifying the constituents of crystals 2B. Identifying lattice parameters 2C. Analyzing crystal systems and structures 2D. Evaluating interatomic interactions 2E. Analyzing symmetry elements
3	Ethical	3A. Using legal software 3B. Transparency in database usage 3C. Responsible for the data analyzed

The respondents were physics students enrolled in a solid-state physics course focusing on crystal structure. The data collection process was conducted using a pre-test and post-test approach, differentiated by the learning methods (Figure 1).

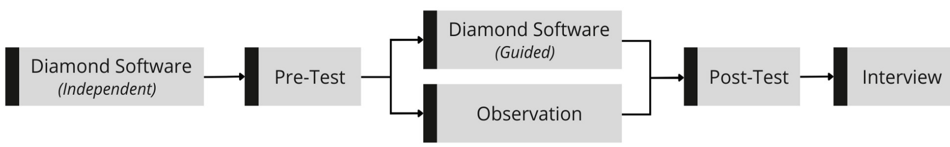

***Figure 1**. Research design*

Each dimension of digital literacy was analyzed separately to identify patterns relevant to the development of students' digital skills. The data were analyzed thematically and classified into several levels of digital literacy adapted from Atmojo's research (Atmojo et al., 2022) as presented in Table 2.

***Table 2**. Category of level literacy digital*

Score	Category
< 30	Very Low
30.00 – 59.99	Low
60.00 – 74.99	Moderate
75.00 – 84.99	High
> 85	Very High

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3 FINDINGS AND DISCUSSION

The research was designed to explore the role of technology, specifically the Diamond software, in visualizing crystal structures to develop students' digital literacy. The enhancement of digital literacy was analyzed based on the technological, cognitive, and ethical dimensions through a pre-test and post-test approach, differentiated by the learning methods, as shown in Figure 1.

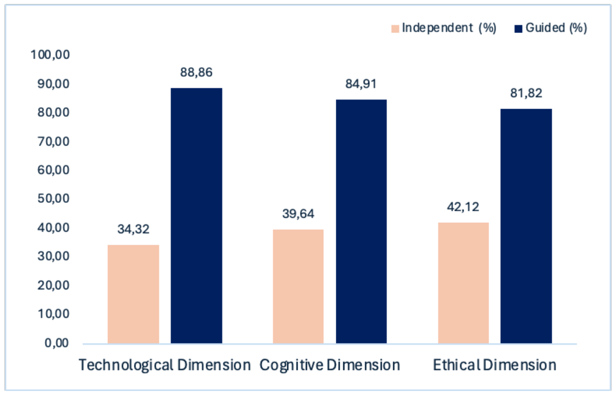

Figure 2. Comparison of digital literacy (pre-test and post-test) based on learning methods

In the technological dimension, the skills of guided students (88.86%) significantly those of independent students (34.32%). This indicated that guidance in using technology was crucial for optimizing students' potential. Cattik & Odluyurt (2017) highlight that guided learning methods greatly influence the enhancement of students' technological skills, particularly in distance learning (Cattik & Odluyurt, 2017). This is further supported by students' statements during the interview session presented in Table 4, where before this, they had never used technology-based media to study crystal structures. They tended to rely on 2D images and text descriptions, which made it difficult for them to use Diamond initially without guidance or other instructions. During the observation session, students showed interest in utilizing various features to study crystal structures, particularly in displaying 3D visualizations, as evidenced by 54.55% increase. These findings align with research by Alakrash (2021), which indicated that the use of technology in education can enhance students' digital literacy (Alakrash & Razak, 2021).

A similar pattern was observed in the cognitive dimension, where students guided exhibit higher compared to those who learn independently. This finding indicated that knowledge and conceptual understanding related to crystal structures were more readily comprehended when instructional support was provided. This was corroborated by Szeto's findings, which assert that interaction between instructors and students during the learning process enhances cognitive understanding, particularly in distance learning (Szeto, 2015). The 45.27% increase in cognitive dimension can also be attributed to students' improved proficiency in operating the Diamond through repeated practice, allowing them to visualize crystal structures more effectively. Thus, the abstract concepts became easier to grasp with the aid of 3D visualization. This was relevant to Saidin's research, which indicates that the use of technology-based learning media can enhance students' understanding of abstract concepts, such as crystal structures (Saidin et al., 2015). Furthermore, in the ethical dimension, although the difference between independent and guided learning was not as pronounced as in other dimensions, guided learning still significantly influences students' ethical awareness regarding technology use (such as Diamond software and crystal databases). This finding emphasizes the importance of teaching ethics in digital literacy (Falloon, 2020).

The use of technology-based visualization tools for crystal structures was not only crucial for deepening students' understanding of complex concepts in distance learning but also as an effective means to enhance students' digital literacy. Interactive visualizations (simulations) enable students to explore microscopic structures more concretely (Eriksen et al., 2020; Pauziah & Laksanawati, 2023) and strengthen critical thinking skills (Syawaludin et al., 2019). Moreover, the use of technology in distance learning is crucial as it facilitates interaction between students and the material without the limitations of physical space (Andreev et al., 2021; Müssig et al., 2020). The combination of technology utilization and guided learning was essential in enhancing students' digital literacy, particularly in distance education, which necessitates rapid adaptation to new technologies (Irdalisa et al., 2020; Müssig et al., 2020).

***Table 3**. Students' digital literacy across each dimension and indicator*

No.	Dimensions	Indicators	Score (%)	Category
1	Technological Dimension	1A	94.55	Very High
		1B	89.09	Very High
		1C	87.27	Very High
		1D	84.55	High
2	Cognitive Dimension	2A	90.91	Very High
		2B	86.36	Very High
		2C	90.00	Very High

		2D	80.91	High
		2E	76.36	High
3	Ethical Dimension	3A	83.64	High
		3B	81.82	High
		3C	80.00	High

The data presented in Table 3 indicate that students exhibit very high proficiency in operating Diamond software (94.55%), processing crystal databases (89.09%), and visualizing 3D crystal (87.27%). These results show that the technological skills improve with more targeted use of the software. Additionally, a high skill level of 84.55% was observed in the aspects of data processing and exporting images or crystal data in specific formats. Müssig et al. (2020) notes that students' experiences with specialized software in online learning can enhance their efficiency in processing crystallographic data. When correlated with the interview results presented in Table 4, it was evident that students still encounter several challenges in using Diamond to visualize crystal structures. In the technological dimension, students require more practice to master the software, indicating that their initial experiences may be insufficient to attain the necessary level of expertise. This inability was also reflected in their limited skills in exploring it.

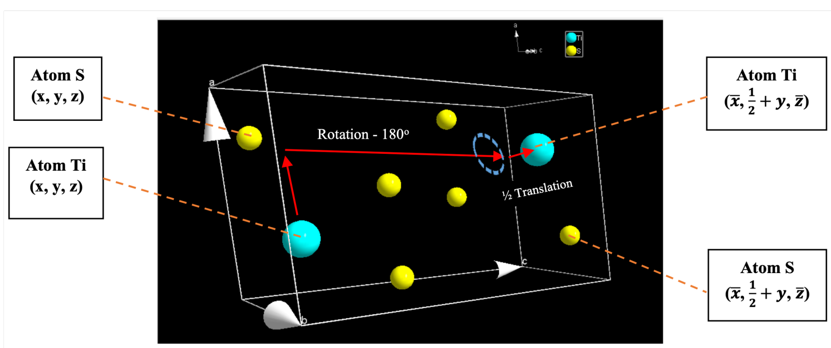

Figure 3*. Crystal structure of the TiS_3 molecule from the COD-1520546 by Diamond Software*

In the cognitive dimension, identifying the constituents of crystals (90.91%) and analyzing crystal systems and structures (90.00%) were very high levels. This indicates that students' understanding of crystal structures improves when they actively engage in analyzing complex data using Diamond software. For example, with the crystal structure of TiS_3 (Figure 3), students can analyze it from various angles, deepening their understanding of atomic arrangements and coordinates within the crystal. This result aligns with previous research indicating that the use of visualization technology can enhance the understanding of complex scientific concepts, such as crystal structures (Casas & Estop, 2015). On the other hand, the lower score of Analyzing symmetry elements (76.36%), suggests that symmetry elements cannot be sufficiently analyzed using only Diamond software, but require additional technologies, specifically designed for symmetry analysis, such as space groups of symmetry through the GESUS application (Miras et al., 2022). The interview results state that students can identify the basic structure of crystals, but they still struggle to analyze complex information, such as crystal planes and symmetry.

***Table 4**. Analysis of digital literacy interviews to the use of Diamond software*

Dimensions	Indicators	Findings	Student' statements
Technological	Basic skills	Students require practice and guidance	"I can perform daily tasks on a computer, but I am new to using this software for visualizing crystal structures. I require more practice and guidance."
	Limited features	Students can only explore basic features	"I can only use the basic features and the existing crystal database to visualize simple crystal structures."
Cognitive	Better visuality	Students can effectively identify the fundamental crystal	"I can more easily see the arrangement of crystal structures, such as atoms and lattices from various angles, especially with the immediate information displayed."
	Analysis difficulties	Students struggle to analyze planes and symmetry	"The crystal image is clear, but I still struggle to analyze complex information, such as the planes and symmetry of the crystal."
Ethical	Source awareness	Students have digital ethical awareness	"I am more aware of the importance of citing data sources and using the software according to its guidelines."
	Responsibility	Students handle crystal responsibly	"Although I still have doubts, I strive to ensure that my visualizations are accurate, especially when presenting them to others."

From an ethical perspective, the aspects of legal software usage and database transparency received scores of 83.64% and 81.82%, respectively. Meanwhile, the responsible for the data analyzed achieved a score of 80.00%, indicating a need for strengthening students' responsibility to interpret and outcomes of their analyses, particularly those intended for publication. This finding is relevant to the interview results (Table 3), which reveal a developing awareness among students regarding the importance of digital ethics, although some hesitation remains in taking full responsibility for data analysis. This finding supports the statement of Elliott K (2021), who asserts that ethical responsibility in data handling greater attention, encompassing not only procedural understanding but also ongoing educational support to ensure consistent comprehension and application (Elliott et al., 2021). Overall, the data concerning the technological, cognitive, and ethical dimensions of learning crystallography are significantly influenced by direct interaction with structured learning platforms. Efforts to enhance digital literacy in distance learning necessitate a more strategic approach to providing technical and instructional support to students.

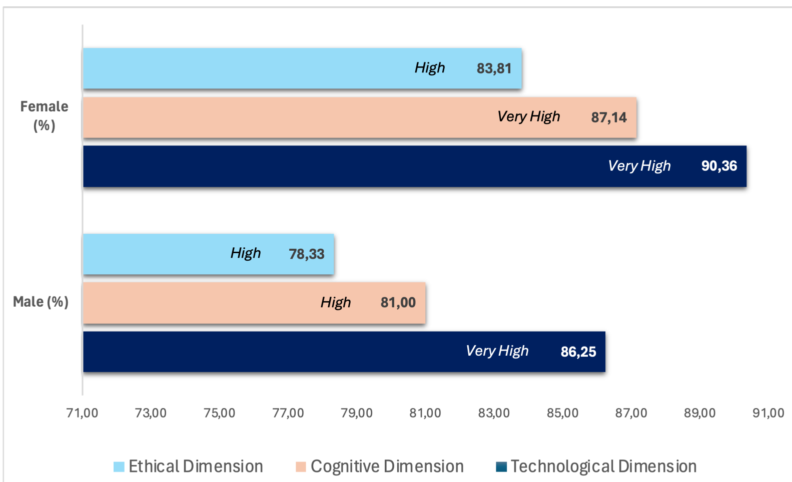

Figure 4. *Digital literacy of students based on gender*

From a gender perspective, the data presented in Figure 4 reveal a notable disparity in digital literacy achievements between male and female students. This difference may be attributed to various factors are environmental, learning motivation, and biological considerations. In the technological dimension, female students demonstrated a slight advantage, with a gap of 4.11%. This finding relevant with research by Park et al (2019), which suggests that visual and technology-based approaches to digital learning are more readily adopted by female students (Park et al., 2019). Despite the perception that females are less engaged with technology compared to males, the data indicate that female participation and motivation in the fields of Science, Technology, Engineering, and Mathematics (STEM) have increased, thereby enhancing their confidence in using technology (Cheryan et al., 2017).

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In the cognitive dimension, the data indicate that females also perform better, with a gap of 6.14%, suggesting that they possess a higher capability in understanding crystallography concepts. Previous research supports these findings, indicating that females possess superior critical thinking skills (Fuad et al., 2017) and exhibit more effective reflective learning styles (Mašić et al., 2020) compared to males, which aids them in comprehending complex information. Furthermore, previous research showed that females tend to follow instructions more closely, more cautious, more comprehensive, and more responsive (Meyers-Levy & Loken, 2015), which explains their advantages in guided learning outcomes. These results are further supported by biological factors, particularly the differences in brain structure, where females possess a larger prefrontal cortex, that area of the brain is crucial for decision-making, problem-solving, and information management, leading females to generally exhibit advantages in verbal abilities and multitasking skills (Hirnstein et al., 2019).

Lastly, in the ethical dimension, both male and female students fall into the "High" category, and females outperform males by a gap of 5.48%. This indicates that female students demonstrate a greater awareness of the appropriate and responsible use of Diamond software by established guidelines. The previous research, females tend to exhibit greater caution in the use of technology (Meyers-Levy & Loken, 2015) and possess higher levels of empathy compared to males (Löffler & Greitemeyer, 2023). This heightened empathy enables them to consider the social and ethical implications of their actions in the digital. Overall, females have shown the performance across all three dimensions of digital literacy. This indicates that women are not only more adaptive to technology use but also more meticulous in analytical and ethical aspects of digital learning in distance learning. Therefore, efforts to enhance digital crystallography education should focus on improving cognitive skills among male students while simultaneously supporting the technological proficiency and ethical awareness of female students. This strategy objectives to reduce the existing gap and promote a more balanced achievement of competencies between both groups.

4 CONCLUSION

Based on the data analysis, the use of the Diamond software as a 3D visualization tool in crystallography education has significantly enhanced students' digital literacy across technological skills (using Diamond Software), cognitive (understanding of crystallography concepts), and ethical (responsibility in using technology, data sources, and analysis results). Pre-test and post-test analyses demonstrate that instructional guidance is effective in optimizing students' abilities to visualize crystal structures, comprehend complex concepts, and enhance ethical awareness regarding technology usage. These findings emphasize the importance of instructional support in technology-based learning, particularly in the visualization of crystal structures within distance learning. Additionally, the analysis identifies a notable difference in digital literacy achievements based on gender, with female students have superior digital literacy.

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