Artificial Intelligence in Sustainable and Green Chemistry Education: A Bibliometric Analysis

Hajidah Salsabila Allissa Fitri, Tiara Swastika Putri, Yuni Hartati Eliya Rosa, and Yuninda Adumiranti

Abstract The integration of Artificial Intelligence (AI) into sustainable and green chemistry education represents a growing interdisciplinary research area that addresses technological advancements and environmental responsibility. This study provides a comprehensive bibliometric analysis of global research trends on AI applications in sustainable and green chemistry education from 2013 to 2025. A total of 56 relevant documents were retrieved from the Scopus database and analyzed using VOSviewer and Biblioshiny. The analysis revealed several prominent research themes: the application of technology and innovation to address sustainability and industrial challenges; the development of AI-based modeling, prediction, and data-driven applications in chemical and environmental processes; the growing attention to researcher roles and the implementation of AI in educational contexts; and critical reflections on the limitations and challenges faced in applying AI to green chemistry education. Co-authorship and keyword co-occurrence networks indicated an emerging, yet still fragmented, collaboration landscape across different countries and institutions. Highly cited articles emphasized the role of AI in enhancing students' conceptual understanding of sustainable chemical practices. These findings suggest that while significant progress has been made in technological integration and environmental modeling, greater efforts are needed to strengthen real-world implementation and to address existing barriers. This study offers valuable insights for researchers, educators, and policymakers seeking to advance sustainable practices in chemistry education through AI innovation.

Keywords Artificial intelligence · Sustainable education · Green chemistry

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1 Introduction

Global issues such as climate change, environmental degradation, and the overexploitation of natural resources have drawn growing attention to the importance of sustainability across various sectors, including education and science [1]. One of the scientific responses to these challenges is the development of green chemistry, an approach in chemical science that focuses on designing products and processes that minimize or eliminate the use and generation of hazardous substances [2–4]. In the educational context, integrating green chemistry principles into the chemistry curriculum and instructional practices has become crucial to fostering environmentally responsible and socially conscious generations of scientists and citizens [5–7].

Aligned with the spirit of sustainable development, chemistry education is expected to go beyond delivering theoretical knowledge by embedding values of sustainability into students' learning experiences [3]. This has led to the emergence of sustainable chemistry education, which combines scientific [8], technological [6], environmental [9], and societal dimensions [10]. This approach encourages students to not only understand chemical reactions or molecular structures but also to think critically about the ecological and societal impacts of chemical practices in real-life contexts [11]. Consequently, educators, curricula, and learning resources must evolve to support meaningful, context-rich learning.

Simultaneously, the rise of emerging digital technologies such as Artificial Intelligence (AI) has transformed the educational landscape [12, 13]. AI enables personalized [14], adaptive [15], and data-driven learning experiences [16]. In the context of chemistry education, AI has been applied in various ways, including intelligent tutoring systems [17], virtual lab simulations [18], data analytics for experiments [19], and interactive learning platforms [20]. These AI applications have shown promise in improving students' understanding of complex concepts [21], supporting differentiated instruction [22], and providing continuous [23], data-informed feedback for both students and educators.

The integration of AI and green chemistry education opens up exciting possibilities for developing instructional approaches that are not only technologically advanced but also environmentally responsible [17]. AI-powered tools can support the modeling of safer chemical processes [24], simulate eco-friendly industrial applications [25], and provide real-time analysis of chemical emissions or waste impacts [26]. However, there is still a scarcity of comprehensive studies that systematically explore how AI is being used specifically in sustainable and green chemistry education.

Bibliometric analysis, as a research method that uses bibliographic data to measure and analyze research trends, will be employed in this study to provide a comprehensive understanding of the development of this interdisciplinary research domain. Through bibliometric tools, this study will identify publication growth, dominant research themes, researcher and institutional collaboration networks, and highly cited literature [27]. This bibliometric approach enables a structured mapping of the conceptual, intellectual, and social dimensions of the literature and offers valuable insights for guiding future research directions.

While bibliometric studies have been widely applied in various fields, including sustainability and educational technology, this study differs by placing a specific focus on the integration of artificial intelligence in sustainable and green chemistry education at a global level. By analyzing publications from 2013 to 2025, this study seeks to answer the following questions: (1) What are the global publication trends and patterns in the field of Artificial Intelligence in Sustainable and Green Chemistry Education over the last decade? (2) What are the most prominent themes, concepts, and keywords that have emerged in the literature? (3) How is the collaboration landscape shaped in terms of authorship networks? It is hoped that this research will contribute meaningful insights for researchers, policymakers, and educators, and to promote collaborative research in building a more innovative and sustainable future for chemistry education.

2 Methodology

2.1 Database Selection and Search Query

To gather relevant literature for the bibliometric analysis, the Scopus database was selected as the primary source of data. Its advanced search capabilities and reliable citation indexing make it particularly suitable for conducting comprehensive bibliometric research. A search query was constructed using a combination of keywords that reflect the focus of this study—artificial intelligence (AI), green or sustainable chemistry, and chemistry education. The Boolean search string used was: TITLE-ABS-KEY ((“artificial intelligence” OR “AI”) AND (“green chemistry” OR “sustainable chemistry”) AND (education OR teaching OR learning OR curriculum OR pedagogy)). The search was limited to documents published between 2013 and 2025, to reflect the recent and emerging nature of the integration of AI in the context of green chemistry education. After executing the query, a total of 56 documents were retrieved from the Scopus database. The inclusion criteria for selecting documents were as follows:

- Articles that contained at least one of the specified keywords in the title, abstract, or keywords.
- Documents written in the English language.
- Document types limited to journal articles and conference papers.
- Subject areas restricted to those relevant to the interdisciplinary scope of this study, particularly education, chemistry, environmental science, and computer science. These fields reflect the integration of educational approaches, chemical sustainability, and artificial intelligence within the context of green chemistry education.

All selected documents were exported in CSV and RIS formats for further analysis using bibliometric software tools.

2.2 Data Analysis

This study employed bibliometric mapping to explore global research trends related to the integration of Artificial Intelligence (AI) in sustainable and green chemistry education. Bibliometric mapping enables the visualization of the structural, conceptual, and intellectual landscape of a research field by identifying relationships among authors, keywords, and publications (Irwanto et al., 2023). To support the analysis, VOSviewer and Biblioshiny (R Bibliometrix package) were utilized as visualization tools. These tools facilitated the examination of citation networks, co-authorship patterns, keyword co-occurrences, and bibliographic coupling (Pabuçcu-Aklş, 2024; Rifqiyah et al., 2024). Through this process, it was possible to identify dominant research themes, collaboration networks, and the evolving scientific domain connecting AI, chemistry education, and sustainability.

This study utilized the Scopus database due to its comprehensive coverage of peer-reviewed literature in science education, technology, environmental sciences, and chemistry. A Boolean search query was designed to capture studies related to artificial intelligence, green/sustainable chemistry, and education: TITLE-ABS-KEY ((“artificial intelligence” OR “AI”) AND (“green chemistry” OR “sustainable chemistry”) AND (education OR teaching OR learning OR curriculum OR pedagogy)).

The search was limited to publications from 2013 to 2025, resulting in 56 documents. Inclusion criteria included: (1) presence of keywords in title, abstract, or keywords; (2) English-language journal articles or conference papers; (3) relevance to education, chemistry, environmental science, or computer science. Selected data were exported in CSV and RIS formats. Bibliometric mapping was conducted to visualize research trends and structures in this interdisciplinary field. VOSviewer and Biblioshiny (R Bibliometrix package) were used to analyze citation networks, co-authorship, keyword co-occurrence, and bibliographic coupling—revealing key themes, author collaborations, and the conceptual landscape connecting AI, sustainability, and chemistry education.

3 Finding and Discussion

The bibliometric mapping conducted in this study offers a comprehensive overview of global research dynamics concerning the integration of artificial intelligence in sustainable and green chemistry education. The results are systematically organized to address three main research questions. First, the publication trends, key contributing countries, institutions, and journals are examined to reveal the growth and geographical distribution of research in this field. Second, keyword co-occurrence and overlay visualizations are analyzed to uncover dominant themes, emerging concepts, and the temporal evolution of scholarly focus. Lastly, collaboration networks are explored through co-authorship to understand the structural patterns and extent of scholarly cooperation.

3.1 Publication Trends Over the Last Decade

The publication trend in the field of artificial intelligence in sustainable and green chemistry education has shown a gradual increase over the past decade. Based on Fig. 1, the number of publications between 2013 and 2020 remained relatively low and stable, with minimal scientific output. A noticeable growth began in 2021, followed by a sharp rise in 2023, reaching its peak in 2024 with the highest number of publications recorded. This upward trend suggests a growing academic and institutional recognition of the importance of integrating AI into sustainable chemistry education. It may also reflect increased funding opportunities and global policy pushes toward digital transformation and green technologies.

Although a slight decline is observed in 2025, this decrease is likely due to the fact that the data collection was conducted only up to April 2025, and therefore does not represent a complete year. Thus, interpretation of trends for 2025 should be made with caution, as the data may not represent the full research activity of the year. The overall trend indicates a significant surge in research interest and scientific activity in recent years. This upward trajectory highlights the growing importance and relevance of integrating AI into sustainable and green chemistry education.

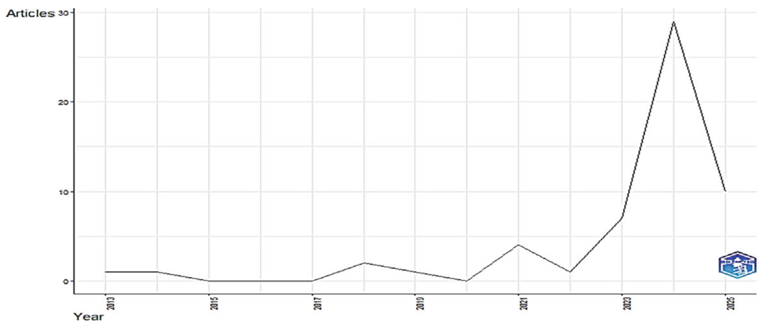

Fig. 1 Annual scientific production

3.2 Key Contributing Countries

As shown in Fig. 2, the analysis of key contributing countries demonstrates the dominant role of the United States (USA), contributing 39 publications, which reflects the country's strong emphasis on technological innovation and sustainable educational initiatives. India follows closely with 38 publications, indicating a strong and growing interest in this area. China ranks third with 27 publications, highlighting its significant role in advancing research at the intersection of AI and sustainable chemistry education. This is notable considering China's global leadership in AI research, suggesting a possible underutilization of these capabilities within chemistry education. Other notable contributors include Saudi Arabia (21 publications), Australia (19 publications), and the United Kingdom (16 publications), demonstrating the global spread of interest in this emerging field. Additionally, countries such as Brazil, Iran, Egypt, Japan, and South Korea also show meaningful contributions, reflecting the international and collaborative nature of research efforts. While the majority of publications are concentrated in a few leading countries, the involvement of diverse regions such as Cameroon, Singapore, and Ethiopia suggests a broadening global participation and an increasing recognition of the importance of sustainable and green chemistry education powered by AI technologies.

This finding indicates that the USA plays a leading role in driving research in this field, possibly due to its strong technological and educational infrastructure. This dominance may reflect the USA's robust investment in STEM education and AI-driven pedagogies. However, it also raises questions about equitable global access to such innovations. It is important to note that the cumulative frequency of publications by country exceeds the total number of articles analyzed. This is because a single publication can be co-authored by researchers from multiple countries, and each contributing country is counted once for each collaborative work. Therefore, the

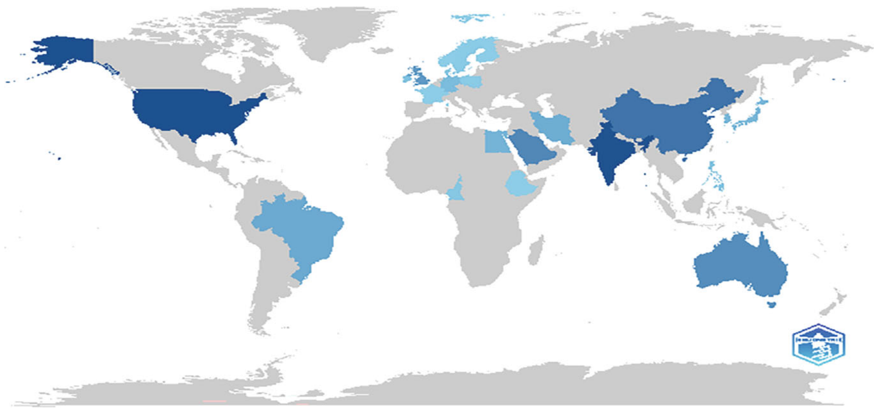

Fig. 2 Country scientific production

figures reflect the collaborative and interconnected nature of research efforts across different nations in this field.

3.3 Most Highly Cited Documents

The analysis of the most highly cited documents and contributing countries provides valuable insights into the global research landscape on the integration of artificial intelligence in sustainable and green chemistry. As shown in Table 1, the United Kingdom leads with a total of 277 citations and an impressive average of 69.2 citations per article, reflecting the strong impact and high quality of research outputs. China and the USA follow with 169 and 119 total citations respectively, although their average citations per article are notably lower. Denmark also stands out, with an average of 31.5 citations per article, highlighting the country's focused and influential contributions to the field. Other countries such as India, Iran, Brazil, Saudi Arabia, Australia, and the Philippines show growing participation, albeit with more modest citation impacts.

Regarding the most highly cited documents as shown in Table 1, the paper by Schweidtmann AM published in Chemical Engineering Journal (2018) is the top-cited publication with 252 citations and an average of 31.5 citations per year, demonstrating its lasting relevance. Following closely, Niazi SK's 2024 paper in Pharmaceuticals achieved 87 citations with an exceptionally high citation rate of 43.5 per year, indicating rapid uptake and influence. Other notable works include those by Jia Y (2021) and Yadav A (2023), showing consistent citation growth. Overall, these

Table 1 Most global cited documents

Paper	DOI	Total citations	TC per year
Schweidtmann AM, 2018, Chem Eng J	https://doi.org/10.1016/j.cej.2018.07.031	252	31.5
Niazi SK, 2024, Pharmaceuticals	https://doi.org/10.3390/ph17010022	87	43.5
Jia Y, 2021, ACS Sustainable Chem Eng	https://doi.org/10.1021/acssuschemeng.1c00483	79	15.8
Yadav A, 2023, Bioresour Technol	https://doi.org/10.1016/j.biortech.2023.129145	68	22.67
Fantke P, 2021, Chem	https://doi.org/10.1016/j.chempr.2021.09.012	57	11.4
Arun M, 2024, Chem Eng J ADV	https://doi.org/10.1016/j.ceja.2024.100589	38	19
Seyyedi SR, 2023, J Environ Manage	https://doi.org/10.1016/j.jenvman.2023.118591	36	12
Leonard KC, 2021, ACS Sustainable Chem Eng	https://doi.org/10.1021/acssuschemeng.1c02741	31	6.2

top-cited documents highlight the increasing academic and industrial importance of artificial intelligence applications in advancing sustainable and green chemistry practices. The increasing citation of studies focusing on sustainable chemistry practices aligns with global efforts outlined in SDG 12, emphasizing the importance of responsible technological integration in education.

4 Keyword Co-occurrence and Thematic Clustering

One of the tools used to analyze the metadata generated from this study is VOSviewer. Figure 3 presents the result of the network visualization and clustering based on the collected documents. The keyword co-occurrence network visualization presents four major clusters that highlight thematic groupings in research intersecting artificial intelligence, sustainable and green chemistry, and education.

The red cluster is the most prominent, consisting of keywords such as technology, integration, sustainability, innovation, industry, challenge, and environmental impact. This cluster reflects a strong focus on the application of technological advancements, particularly AI, in addressing industrial and sustainability-related challenges. It suggests that researchers have placed substantial emphasis on how technology and innovation contribute to the optimization and integration of sustainable practices in chemistry.

The green cluster includes keywords such as model, application, development, data, environment, prediction, chemical, use, and temperature. This cluster indicates that a significant body of research is dedicated to AI-based modeling, prediction, and data-driven applications in the field of green chemistry. The co-occurrence of terms like chemical, model, and prediction suggests a strong link between computational

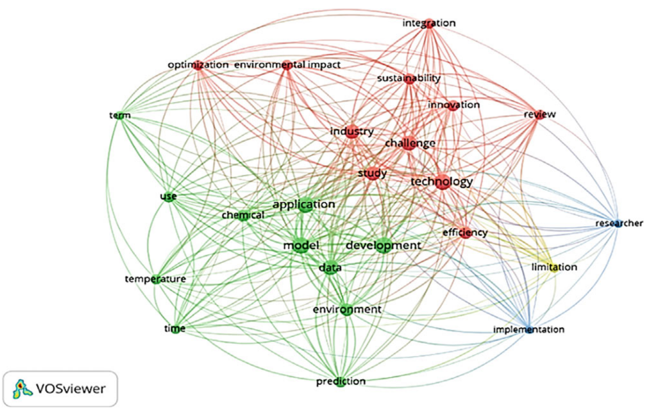

Fig. 3 Network visualization

approaches and environmental analysis, reinforcing the role of AI in improving the precision and environmental performance of chemical processes.

In contrast, the blue cluster is smaller and consists of researcher and implementation. This implies a growing but still limited attention to the role of researchers and the actual implementation of AI in sustainable chemistry education. The presence of implementation as a bridging node might reflect ongoing efforts to move from conceptual frameworks toward real-world application, although this domain remains underexplored.

Meanwhile, the yellow cluster is represented by a single keyword, limitation, which highlights critical reflections on the constraints or barriers encountered in the application of AI in this field. This could include technological limitations, pedagogical gaps, or institutional challenges that need to be addressed to fully realize the potential of AI in green chemistry education.

Analysis of keywords used by authors in publications is an essential tool for investigating trending topics and research focus in the field. Publication keywords quickly highlight the themes and areas of emphasis within scholarly works. The WordCloud in Fig. 4 illustrates the most frequently used keywords in publications related to the intersection of Artificial Intelligence, Machine Learning, and Green Chemistry. The data indicates that "machine learning" and "artificial intelligence" are dominant topics, appearing 45 and 39 times respectively, reflecting a major research trend toward integrating advanced computational techniques in sustainable practices. This suggests that machine learning and artificial intelligence are becoming a central methodology in green chemistry education research. Additionally, terms such as "green chemistry," "sustainable chemistry," and "sustainable development" emphasize a growing commitment to environmental sustainability through innovative technologies. Human-centered research also features prominently, highlighting ethical considerations and applications in real-world contexts.

As shown in Fig. 4, the keywords "machine learning" and "artificial intelligence" have been prominent terms with consistent and significant presence in the analyzed

Fig. 4 Word cloud

publications. This suggests an ongoing and growing interest in the application of these technologies within sustainable and green chemistry contexts. "Machine learning" appears as the most frequently used keyword, followed closely by "artificial intelligence," indicating their central role in driving innovation and research in this field.

Recent studies have highlighted that the integration of machine learning and artificial intelligence can significantly enhance predictive modeling, optimization, and efficiency in sustainable chemical processes. This indicates a sustained and increasing importance of these technologies, reflecting their transformative impact on research and industrial practices toward achieving sustainability goals. The limited presence of education-focused keywords suggests that although AI applications in green chemistry are rapidly evolving, their incorporation specifically into educational frameworks remains a developing subfield. This suggests that while AI is gaining traction in green chemistry, its pedagogical implementation is still under-researched. Future studies could explore how AI-enhanced tools are actually used in classroom practice.

4.1 Evolution of Keywords Over Time

The overlay visualization map (as presented in Fig. 5) provides a temporal perspective on the evolution of keywords related to the integration of artificial intelligence (AI) in sustainable and green chemistry education. This map illustrates the average publication year of each keyword using a color gradient ranging from dark blue (older terms, around 2022) to yellow (newer terms, approaching 2024).

Keywords such as "chemical," "model," "data," and "prediction" are mostly colored in shades of blue and green, indicating their early appearance in the dataset

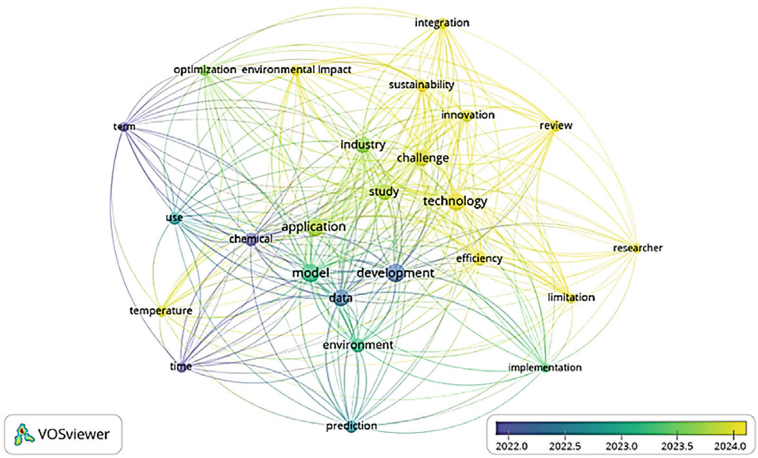

Fig. 5 Overlay Visualization

and their foundational role in the earlier stages of the research field. These terms are typically associated with the technical and computational aspects of integrating AI in chemistry education.

In contrast, more recent terms like “technology,” “innovation,” “integration,” “review,” and “researcher” are displayed in yellow, suggesting a shift in research focus toward broader themes such as the practical implementation of AI technologies, critical evaluations, and interdisciplinary integration. This shift reflects an increasing interest in the application, reflection, and evaluation of AI within educational and sustainable chemistry contexts.

Furthermore, the appearance of terms like “sustainability,” “environmental impact,” and “challenge” in yellow also highlights growing concerns and discussions around the real-world implications and societal relevance of AI-enhanced education in chemistry. In summary, this overlay visualization not only emphasizes the chronological development of research themes but also captures the dynamic evolution from foundational computational concepts to broader, more reflective, and interdisciplinary perspectives.

4.2 Co-authorship Network Analysis

In this section, we analyzed the co-authorship and bibliographic coupling networks of the authors in the dataset. The visualization of the co-authorship network, as shown in Fig. 6, illustrates collaboration patterns among researchers. Each cluster is represented with a different color, indicating separate groups of collaboration. From the visualization, it is evident that the largest cluster, depicted in gray, is formed by Almutairy BK, Abourerejab MAS, and Alfadhel MM, who demonstrate strong collaboration ties. Other smaller clusters, such as those led by Lapkin AA, Alhuqail AA, and Ramakrishna S, indicate more localized research partnerships. Each node’s size reflects the number of documents produced by the author, while the lines connecting nodes represent co-authorship links. Overall, the network structure reveals relatively independent clusters with limited interconnection between groups, suggesting that collaboration within this research field is fragmented and often confined within small, tightly connected groups of two to three authors.

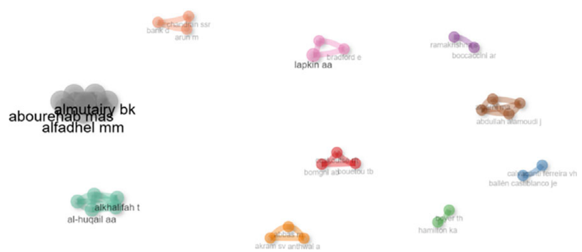

Fig. 6 Collaboration between author

5 Conclusion and Recommendation

This bibliometric analysis shows that research activity has notably increased since 2021, peaking in 2024, indicating growing interest driven by digitalization and sustainability trends. Thematic clustering revealed four focal areas: technological integration, AI-based modeling, implementation challenges, and limitations—highlighted by keywords such as machine learning, artificial intelligence, and green chemistry. Co-authorship patterns show strong contributions from the US, India, and China, with key institutions including the Center for Computational Toxicology and Exposure, University of Campinas, and National Kaohsiung University of Science and Technology. However, geographic concentration remains high, signaling a need for more inclusive global engagement. Future studies should foster interdisciplinary collaboration across AI, green chemistry, and education, especially involving underrepresented regions. Researchers are encouraged to develop practical, scalable models that bridge theory with real-world application, while addressing systemic barriers to optimize AI's role in promoting sustainable chemistry education.

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