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Qualitative Study on Integration of Artificial Intelligence Tools in Chemistry Education Programs and Research for Sustainable Development in Nigeria

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Abstract
This study explores the integration of artificial intelligence (AI) tools into chemistry education and research with a focus on sustainable development. The objectives for this theoretical work were towards integrating AI tools in chemistry education and research. Nine processes of AI were juxtaposed from literature to actualise the objectives in this article viz: computer simulation for chemistry education programs; virtual laboratory for chemistry education program; personalised learning for chemistry education program; automated assessment for chemistry education program; integration of AI tools in organic synthesis; integration of AI tools in molecular designing; integration of AI tools in detection of molecular properties; integration of AI tools in spectroscopy and analytical methods and integration of AI tools in waste water treatment. The overview of current knowledge on this topic was achieved through relevant literature. The paper also examines the challenges of AI in chemistry education which include data quality, model validation, ethics and security. The study recommends that professional development programs should be organized to enhance teachers' confidence and competence in implementing AI tools in their classrooms thereby enriching the learning experience.
Keywords: Artificial intelligence, chemistry education and sustainable development

Introduction
Artificial intelligence (AI) is a computer software that works like human brain and can do difficult tasks such as being able to see, understand, and respond to spoken or written language, analyse data, make recommendations and more (Maslej *et al.,* 2023). This system is used to make obtainable breakthroughs in medicine, education and research to uncover secrets long hidden from human knowledge. AI allows users to think more quickly, make faster decisions and provide more practical and solutions (Swoope, 2020). Intelligence has been considered as one of the most important qualities of human beings because every human behavior has actually been described to intelligence (Robinson, 2018). AI has become the main catalyst in drastic transformation in various fields of science one of which is chemistry. In the field of chemistry education and research, AI provides opportunities to overcome long – standing challenges such as limited laboratory infrastructure, high cost of reagents, and inadequate access to research facilities particularly in developing countries like Nigeria. By integrating AI powered tools such as virtual laboratories, intelligent tutoring systems, and data - driven modelling, chemistry education can become more inclusive, cost - effective, and aligned with the principle of sustainable development.

The advent of AI has profoundly impacted the field of chemistry education (Cetin - Dindar *et al.,* 2018). It enhances experimental accuracy and further facilitates comprehensive understanding of complex concepts, advanced research methodologies and more rapid data interpretation (Ali and Ula, 2020; Swoope, 2020). This study therefore explores the way AI tools can be harnessed to transform chemistry teaching, learning and research in Nigeria where access to functional laboratories, modern research infrastructure and quality educational resources is limited (UNESCO, 2021). Conceptually, AI integration is framed as a bridge between the persistent challenges of chemistry education in Nigeria and the desired sustainable outcomes (enhanced learning innovation, and environmentally responsible research practices). This article provided theoretical analysis of how AI tools would support teaching, learning and research for sustainable development. Further search into literature helps to explore contemporary research on how integration of AI into chemistry education programs would help in enhancing the pedagogy of the subject. The objectives for preparing this review were towards integrating AI tools in chemistry education program towards meeting sustainable development. The following theoretical analyses were explored from literature for developing the specific roles which AI plays in enhancing chemistry teaching and learning and are listed and discussed as follows: Computer Simulation for Chemistry; Education Program; Virtual Laboratory for Chemistry Education Program; Personalised Learning for Chemistry Education Program; Automated Assessment for Chemistry Education Program; Integration of AI tools in organic synthesis; Integration of AI tools in molecular designing; Integration of AI tools in detection of molecular properties; Integration of AI tools in spectroscopy and analytical methods; Integration of AI tools in waste water treatment**.**

Computer Simulation for Chemistry Education Program

Chemistry involves microscopic concepts that are often abstract and difficult to comprehend (Taber, 2018). Traditional laboratory experiments can also be expensive, hazardous, or inaccessible in some schools. Therefore, the need for integrating computer simulation tool in the teaching and learning the subject at all levels of education arises. Computer simulation is a computer program that creates animated, interactive, game - like environments which focus on connecting real life phenomena to the underlying science (Oladejo *et al.,* 2021). Within this process, it makes the visual and conceptual models designed by experts and scientists simple, so that they can be understood by learners. In chemistry education, simulation provide learners with opportunities to visualise molecular interactions, conduct virtual experiments, and test hypothesis in a safe and cost-effective environment. The study conducted by Suratno and Aydawati (2017), Salame and Makki (2021), Almasri (2022) show that simulation help students to learn difficult chemistry topics, because it provides visual representation of complex systems and abstract concepts that are really hard to understand. For instance, simulations show how atoms and molecules interact with each other. The study further recommended that computer simulations are powerful tool for chemistry education, as they provide students with a dynamic and interactive learning environment that complement what has been difficult to understand in the traditional teaching method.

It is a useful facility for improving students' performance in chemistry and promoting meaningful learning (Jane *et al.,* 2017; Oladejo *et al.,* 2021, Salome *et al.,* 2023). It assisted learners to be more creative and innovative in chemistry than the traditional methods that over depends on teacher expertise and teaching skills. According to Jane *et al.,* 2017 and Beichumila *et al.,* 2022, examples of chemistry topics well suited for simulation include: Molecular models: visualizing the structure and bonding of molecules; Chemical kinetics: Exploring the kinetics and mechanisms of chemical reactions; Electrochemistry: presenting dynamic nature of the process; Phase changes: simulating the behavior of matter in different states; Thermodynamics: Exploring energy transfer and equilibrium; Organic chemistry: Visualizing reaction pathways and mechanisms; Spectroscopy: Exploring the interaction of electromagnetic radiation with matter

Virtual Laboratory for Chemistry Education Program

Virtual laboratory in chemistry refers to computer - based simulation of laboratory experiments that enable users to conduct scientific experiments or activities in a digital environment (via computer software, internet platforms, or mobile applications) without physical laboratory infrastructure (Phang *et al.,* 2024). Virtual laboratories serve as platforms for students to stimulate real- world problems and reactions in a virtual environment (Mutlu and Acar Sesen, 2016). They also offer interactive elements that allow learners to manipulate variables, observe outcomes, analyse data, flexibility to repeat experiments and interact with various aspects of the experiment, thus fostering a deeper understanding of the concepts. Many researchers reported positive impact on the use of virtual labs in the teaching and learning chemistry (Zhu and Liu, 2020; Kafilan *et al.,* 2021; Alhashem and Alfailakawi, 2023, Faralla *et al.,* 2024).

In chemistry education program, virtual laboratories are particularly useful for improving engagement and personalised learning. They allow students to repeat experiments multiple times, adjust learning pace, and explore beyond the constraints of time and resources (Makransky *et al.,* 2016). In addition, integration of virtual laboratories into curricula has been shown to increase students' problem-solving skills, motivation, and academic performance (Raman *et al.,* 2020). In the Nigerian context, where access to well-equipped laboratories is often limited, virtual laboratories can play a crucial role in expanding opportunities in science education. By combining virtual laboratories with traditional laboratories in a blended approach, institutions can provide students with both theoretical grounding and practical exposure (Penn and Ramnarain, 2019). This aligns with global trends in digital education and supports the sustainable development goal (SDG 4) on quality education.

Personalized Learning for Chemistry Education Program

Personalized learning instructional strategy is a type of teaching strategy that takes care of individual differences since the students are allowed to learn at their face, cognitive style, strategy among others (Guyah *et al.,* 2021). According to

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Cardenas *et al.,* (2021), personalized learning refers to an instructional approach that tailors educational experiences to individual students' prior knowledge, needs, capacities and perceptions during the teaching -learning processes to adapt future contents to their identified learning requirements, problems or needs. In chemistry education programs, personalised learning integrates digital technologies, adaptive platforms, and learner – centered strategies to provide flexible pathways for mastering complex scientific concepts (Pane, *et al.,* 2015). Chemistry, being a subject that requires both conceptual understanding and practical application, benefits significantly from personalised learning. Digital tools such as adaptive simulations intelligent tutoring systems, and virtual laboratories allow students to learn at their own pace and revisit challenging concepts until mastery is achieved (Ilic, *et al.,* 2024). This approach accommodates diverse learners and helps to reduce achievement gaps often seen in science classrooms. Personalised learning enhances learners' engagement by allowing them to explore topics at their own pace and based on their interests. According to pane *et al.,* (2017), students in personalised learning environments reported higher level of motivation and ownership of their learning compared to those in traditional classrooms. It also accommodates diverse learning need, including those of students with disabilities and varying learning styles. Basam *et al.,* (2016) observed that personalised learning fosters inclusivity by integrating adaptive technologies and differentiated instruction. In the Nigerian context, personalised learning has the potential to address challenges such as overcrowded classrooms, limited laboratory resources and varying student preparedness. By integrating personalized learning with computer simulations and e - learning platforms, chemistry education can become more inclusive, efficient, and impactful (Okebukola, 2020). Moreover, this allingns with global trends towards digital transformation in education and supports the sustainable development goals (SDG 4) on equitable quality education.

Automated Assessment for Chemistry Education Program

Automated assessment is a modern form of assessment that makes use of technology in planning developing, administering and scoring assessment. It relies heavily on technology to streamline all forms of activities that will lead to students learning performance within the school setting. It involves the use of technological tools such as large language model in developing multiple -choice items (Chen *et al.,* 2020). In chemistry education programs, automated assessment is increasingly used to grade assignments, laboratory reports, quizzes, and even simulations, thereby enhancing efficiency and consistency in evaluation (Gamage *et al.,2019*). The need for change from traditional assessment strategies to automated assessment arises due to the advancement in information and telecommunication technology. This led to the utilisation of automated test items, especially the objective related like multiple choice that have the options out which computers can identify the correct options with ease and saving of time though the assessment standard does not change (Ewim and Opateye, 2021). One of the major advantages of automated assessment in chemistry is consistency and fairness. Unlike human grading, which can be influenced by fatigue, automated assessment applies the same criteria uniformly, ensuring fair marking across all students (Nguyen *et al.,* 2020)

In the context of practical chemistry, emerging technologies such as virtual laboratories and computer simulations integrate automated assessment to evaluate experimental design procedural accuracy and interpretation of results (Tatli and Ayas, 2013). These systems can measure not only cognitive outcomes but also process skills such as data handling and analytical reasoning. One of the challenges of automated assessment is that automated systems depend on algorithms and databases. If not well - programmed, they may incorrectly mark partially correct answers (e. g. molecular structures, chemical equations with minor formatting differences) as wrong (Gupta and Pathania, 2021).

Integration of AI tools in Organic Synthesis

Organic synthesis encompasses a vast number of reactions, traditionally necessitating extensive experimentation to determine optical reaction conditions. However, machine learning algorithms can identify patterns from extensive reaction datasets enabling the prediction of novel reaction outcomes (Hein, 2021). This not only saves time and resources but also facilitates the discovery of new reaction conditions (Gromski, *et al.,* 2019). Furthermore, AI can be employed for the optimization of reaction conditions, maximizing reaction yield and selectivity (Gao *et al.,* 2018), by analyzing a wealth of experimental data, machine learning algorithms identify optimal reaction conditions, assisting chemists in designing experiments more effectively (Taylor, *et al.,* 2023).

Integration of AI tools in Molecular Designing

AI plays a crucial role in molecular designing by accelerating the process of identifying and designing molecules with specific properties, particularly in drug discovery and development. Drug discovery includes the intricate process of designing, identifying and developing new medications aimed at improving human health and combating diseases. Traditionally this process has demanded significant time (averagely 12 years) and cost which at the end results in persistent challenges in addressing chronic diseases such as diabetes and cancers (Perron *et al.,* 2022). The advent of AI marks a revolutionary shift in drug development, offering a suite of advanced computational tools designed to augment human capabilities rather than replace them (Anstine and Isayev, 2023). At its core AI leverages sophisticated algorithms for autonomous decision making from data analysis revolutionizing the pharmaceutical land scape (Al - Sarayreh *et al.,* 2023). Molecular design is the creation of novel molecules with desired properties for a given problem in chemistry, material science or nanotechnology (Loeffler, *et al.,* 2024). According to Puri *et al.,* (2024), the use of AI and machine learning can help to optimise chemical reactions or enhance precision and reduce time consume for chemical reactions and this key can help one progress in designing drugs and pharmaceutical technology.

Integration of AI tools in Detection of molecular properties

In addition to the traditional wet lab method, researchers have also developed numerous AI models for predicting molecular properties (Shen and Nicolaou, 2020). AI algorithms can analyse chemical data to predict and classify various molecular properties such as toxicity, solubility and reactivity. This makes the process of detection faster and less prone to errors unlike manual detection. Moreover, AI allows scientist to evaluate the potential of a hypothetical molecule.

Integration of AI tools in Spectroscopy and Analytical Method Development

The application of AI in the interpretation of spectroscopic data has become a rapidly expanding field of research, owing to its ability to extract meaningful information from complex data sets. Spectroscopy, which involves the measurement and interpretation of the interaction between matter and electromagnetic radiation, generates large volumes of data that can be challenging to analyse manually (Rial *et al.,* 2024). In analytical chemistry, AI is revolutionizing the approach to complex data analysis and the development of innovative methods. AI's capabilities in interpreting large data volumes and automating analyses enhance efficiency, accuracy and reliability in the field (Prasad and Kalpana, 2024).

Integration of AI tools in Waste water treatment

Traditional methods of waste water treatment often face limitations in terms of effectiveness, energy consumption and cost efficiency (Wang *et al.,* 2019). The integration technologies offer a new model for addressing these challenges by enhancing efficiency, accuracy and automation of waste water treatment processes by using machine learning algorithms, predicting modelling methodologies and sophisticated analytics. AI can optimise various aspects of wastewater treatment, including pollutant detection, process control resource recovery and system optimisation (Obardeen *et al.,* 2023). It helps in the treatment of wastewater by taking the data from biological stage. This data provides a prediction based on the behavior of bioreactor. It provides the operation that is useful in waste water treatment. This AI based system is more efficient than the human understanding in waste water treatment plant. This technique implements some algorithms to make the analysis more intelligible (Choudhary *et al.,* 2022). AI is a key enabling technology in the journey toward sustainability. It is the most important part of the technology industry because it helps in collecting and analyzing data at a low cost and having a safe working environment. It has been fundamental in addressing pollution control, renewable energy development and green chemistry initiatives. The sustainable development goals (SDGs), established by the United Nations provide a road map for achieving sustainable development by the year 2030 (Gulseven, 2020).

Challenges of integrating AI technology in the Development of Chemistry Education

According to Akbar and Djakariah (2024), some of the challenges for AI applications in education, include:

i. Data quality: The quality and quantity of relevant chemical data is often a challenge. Sometimes, available datasets are limited in coverage or diversity, which can affect the accuracy and generalization of the models built.
ii. Model validation. Complex models are often difficult to interpret. This can be a problem in chemistry where the importance of understanding molecular structure and interactions is key.
iii. Ethics and security: Sensitive data in chemistry research must be kept secure, especially when using AI techniques that require access to sensitive data or valuable experiments. The use of AI in chemistry learning also raises ethical questions about the responsible use of this technology especially in its use for the development of new drugs or chemicals.

Collaborations between chemists, computer scientists and AI experts is required in addressing these challenges to overcome limitations, improve interpretability, and ensure safety and ethics in the application of AI in chemistry learning.

Conclusion

AI plays important role in chemistry education and research in various ways. It revolutionizes conventional teaching methodologies to innovative teaching method which provide interactive and engaging learning experience that can help students build their knowledge more effectively. In chemical research, AI serves as a powerful tool in enhancing efficiency and expediting research, discovery and innovation in sustainable chemical processes.

Recommendations

1. Government and non - governmental organizations (NGOs) should assist in providing the facilities required for AI implementations.
2. Professional development programs should be organized to enhance teachers' confidence and competence in implementing AI tools in their classrooms thereby enriching the learning experience.
3. Challenges associated with the application of AI in educational sector, such as lack of monetary resource, lack of interest on the part of institution administration and lack of knowledge about successful involvement in the field should be addressed.

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