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AI in chemistry and chemical education

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Abstract

Artificial Intelligence (AI) is reshaping chemistry education by offering new tools for teaching, learning, and research. We explore how AI can both support chemistry learning and serve as a subject of instruction, while also addressing the ethical, technical, and educational challenges involved. It highlights the need to systematically integrate AI-related competencies into teacher education, guided by frameworks like DiKoLAN AI. A reflective, responsible approach is essential to ensure that AI enhances, rather than undermines, scientific understanding and equity in the classroom.

Keywords

Artificial intelligence, chemical education, AI

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Introduction

Artificial Intelligence is no longer just transforming research labs — it's making its way into classrooms, reshaping the way we teach, learn, and understand chemistry. As AI becomes an essential part of modern scientific practice, chemistry education faces an exciting challenge: how to equip students and teachers with the skills to thrive in an AI-enhanced scientific world. From predictive models for chemical reactions to intelligent tutoring systems that adapt to individual learning needs, AI offers powerful new tools to support both learners and educators. At the same time, it raises important questions: How can we teach students to understand and critically assess AI-driven insights? How do we prepare future chemistry teachers to use AI responsibly and effectively in their classrooms?

This proposal explores the role of AI in chemistry education — as both a subject of learning and a transformative teaching tool. It outlines the opportunities, risks, and necessary competencies to ensure that AI enhances, rather than replaces, meaningful scientific learning and teaching. In general, it's clear that we should cultivate awareness of AI in all areas of life — for instance, did you notice that this introduction was written with the help of ChatGPT?

AI in chemistry

Recent advancements in AI research have significantly impacted various professional fields and society at large, introducing both novel opportunities and challenges. These developments have profoundly influenced key aspects of everyday life, including healthcare (Dunn et al., 2023; Jindal et al., 2024), finance (OECD, 2023), and mobility (Craglia et al., 2021).

Beyond its role in everyday life, Artificial Intelligence (AI) is also increasingly important in scientific research and applications (Berber et al., 2025). In 2023, AI was already counted among the most important emerging technologies in chemical research (Gomollón-Bel, 2023). The ability to process large amounts of data more efficiently using machine learning and neural networks is permanently changing the way modern scientific research is done and enabling previously unimaginable scientific advances to be made.

The awarding of the 2024 Nobel Prize in Chemistry for the development of AlphaFold and its contributions to protein structure prediction further underscores the transformative impact of AI on modern science research and applications (The Royal Swedish Academy of Sciences, 2024). AlphaFold plays a revolutionary role, as it was able to predict the spatial structure of all previously known proteins starting from the primary structure with astonishing accuracy in no time. Consequently, the understanding of the function and regulatory possibilities of a large number of proteins is supported, which represents a major advance for areas such as pharmacology (Jumper et al., 2021). At the same time, AI is increasingly aiding the synthesis of complex drug molecules, enabling the identification of novel synthetic routes and improving the efficiency of already established paths (e.g. Ishida et al., 2022).

In addition to the main areas of chemical research, AI is also finding its way into other chemistry-related sciences such as cell biology, medicine and materials science, as well as other areas of scientific research such as astrophysics and high-energy physics. The analysis of image data, modeling of molecules and particle interactions as well as the prediction of material properties make it possible to pose new research questions and realize corresponding research projects (e.g. Liu et al., 2023; Lourenço et al., 2023).

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In Conclusion, AI's integration in science already spans a wide range of research domains and highlights both the immense potential and the associated risks and challenges of AI technologies.

AI in chemistry education

Overall, technological development and the integration of AI are leading to social and professional changes. According to the World Economic Forum (Battista et al., 2025), technology-related professions such as AI and machine learning specialists are the fastest-growing job sector.
In view of AI's individual and social relevance and the wide range of possible applications, there is a clear mandate to promote AI skills. This mandate goes beyond empowering citizens to engage in an increasingly AI-driven society (Touretzky et al., 2019; UNESCO, 2022); it also includes preparing younger generations specifically for the changing landscape of chemistry education and science education in general (Döbeli Honegger, 2016). This mission includes exploring and systematically integrating AI applications in science into school and university curricula.

Learning about AI in in the Chemistry Classroom

Integrating artificial intelligence (AI) as a learning object in chemistry lessons enables students to develop a basic understanding of the functioning and application of AI in the natural sciences and to see AI-based methods as part of chemical work and research. Studies show that such technologies can increase learners' interest and improve their analytical skills (Jiang et al., 2023). In addition, engaging with AI in chemistry lessons enables critical reflection on the role of algorithms in scientific processes. Students can learn how AI is used to analyze complex chemical data (big data) and what limits and possibilities are associated with it. This can help to develop an understanding of modern scientific methods and promote media literacy and critical thinking.

Learning with AI in chemistry lessons

AI can also be an effective learning tool and companion in chemistry lessons. Adaptive learning systems based on AI enable individual student support by adapting content to the respective performance level individually and in real-time (Maier & Klotz, 2022).
AI can help teachers to plan, implement and reflect on lessons efficiently and "*respond better to individual learning needs*". This includes, for example, the use of AI chatbots and intelligent tutoring systems (ITS) in lessons to make them adaptive through individual diagnostics and scaffolding (e.g. Mousavinasab et al., 2021). In addition, the AI-supported generation of learning materials (e.g. Sarsa et al., 2022) allows teachers to have more time available for individual support of students.

Ethical implications

The use of AI in chemistry lessons raises various ethical questions. One key concern relates to the potential digital isolation of learners. If AI systems replace human interactions, this could lead to a decrease in social learning, which is essential for the development of communicative and cooperative skills.
Another ethical concern is the transparency and traceability of AI-supported decisions in education. It is important that students and teachers understand how AI systems work and on what basis they make recommendations or assessments. This requires appropriate education and training in the use of AI technologies and thus the development of subject-specific AI literacy.

Risks and challenges

Not all schools have the necessary resources to use AI-supported tools in chemistry lessons. This can lead to a digital divide where students in less equipped schools are disadvantaged. It is therefore important to ensure equitable access to technological educational resources.

The use of AI in chemistry lessons requires the collection and processing of students' personal data. This raises data protection issues, particularly with regard to compliance with the EU's General Data Protection Regulation (DSGVO). It is crucial that schools and educational institutions implement transparent data protection policies and obtain consent from data subjects.

AI systems can have biases that negatively impact the learning process. Typical misconceptions and explanatory biases on chemical topics are partly reproduced by AI (Talanquer, 2023). These can have a direct impact on the learning processes of students and can consolidate their own misconceptions. Furthermore, gender and racial biases are present, for example, in the portrayal of chemists (Kaufenberg-Lashua et al., 2024). People with visible disabilities are strongly underrepresented by AI (Kaufenberg-Lashua et al., 2024). If training data is not representative, certain groups of students may be disadvantaged and not able to identify with people like chemists. It is therefore important to regularly check AI systems for bias and misconceptions and make appropriate corrections.

Excessive use of AI in the classroom could lead to students' basic skills, such as critical thinking and problem-solving skills, being neglected. However, critical thinking skills in particular are essential for dealing with AI in the classroom (Blonder & Feldman-Maggor, 2024). This so-called "skill-killing" can affect learners' independence and increase their dependence on technology.

Finally, there are regulatory challenges, such as the EU's AI Act. This places new requirements on the use of AI systems, particularly in sensitive areas such as education. Schools must therefore ensure that the AI applications used comply with these legal requirements.

AI in chemistry teacher education

However, to effectively teach AI within subject-specific contexts or to utilize it as a tool for lesson planning and follow-up, teachers must possess the necessary AI-related competencies. This necessitates a targeted adaptation of teacher education by systematically and structurally embedding AI-related skills into both initial teacher training and continuing professional development programs.

The integration of artificial intelligence (AI) into the training of chemistry teachers is essential if the potentials, opportunities, risks, and challenges described above are to be adequately integrated

into the chemistry classroom. There are existing frameworks that can be used to integrate technology into teacher training:
One framework that describes digital competency domains for teachers is the TPACK model (Koehler, Mishra, & Cain, 2013). However, this framework reaches its limits when covering implications and transformations of and by AI in all areas of life and work, especially in chemistry (Mishra, Warr, & Islam, 2023).

In science education, the DPACK model (Digitality-Related Pedagogical and Content Knowledge) by Thyssen et al. (2023) extends the well-known TPACK model. It takes into account the specific requirements of digital technologies and emphasizes the need to include socio-cultural aspects, e.g., covering things like human-machine interactions.

The UNESCO AI Competency Framework for Teachers (2024) is specific to AI competencies. This identifies five key areas of competence: a human-centered mindset, ethics of AI, foundations, and applications of AI, AI pedagogy, and AI for professional development. These competencies are designed to enable teachers to integrate AI responsibly and effectively into educational processes. The framework emphasizes the importance of ethical principles, such as fairness, transparency, and privacy. It underlines the need to view AI as a supporting tool that complements, not replaces, the role of the teacher. However, the framework lacks a focus on a specific subject, such as chemistry.

The DiKoLAN AI framework (Huwer et al., 2024) is an extension of the original DiKoLAN framework (Digitale Kompetenzen für das Lehramt in den Naturwissenschaften)(von Kotzebue et al., 2021), which is specifically tailored to the requirements of teaching with and about artificial intelligence (AI). The aim is to provide prospective and practicing teachers with a structured orientation framework to integrate AI competencies into teacher education systematically. In contrast to a separate category for AI competencies, the DiKoLAN AI model integrates AI-related skills into existing competence areas of the DiKoLAN framework. This includes, for example, the ability to use AI-supported simulations in science lessons, to reflect on ethical aspects of AI applications, and to use AI technologies in a didactically meaningful way. The DiKoLAN AI competency model serves as the basis for developing curricula, training programs, and teaching materials that prepare teachers for the effective and reflective use of AI in science lessons.

The task therefore remains of successively integrating the specific competencies for chemistry teachers already formulated in the DiKoLAN AI framework into teacher training and developing specific courses.

Conclusions

Artificial intelligence holds high relevance and offers a wide range of applications in chemical research, making it increasingly important in both individual and societal contexts. To prepare students for the future, it is essential to integrate and promote AI-related skills also within chemistry education. This includes not only learning about AI applications but additionally using AI as a learning tool and companion in the classroom. However, the integration of AI framework presents challenges, such as ethical concerns, varying levels of access and digital preparedness, and the risk of biased algorithms. Therefore, a reflective and purposeful use of AI in chemistry education—aligned with legal and ethical guidelines—is necessary. A key prerequisite for this is the development of AI-related competencies among teachers. To achieve this, AI should be meaningfully incorporated into teacher training programs, guided by frameworks such as the DiKoLAN AI framework. Therefore, the International Journal of Physics and Chemistry Education invites submissions for papers dedicated to Artificial Intelligence in the science classroom. IJPCE welcomes original research, case studies, reviews, and theoretical contributions that explore the integration of AI in science education.

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