



# Review on ChatGPT: History, Applications and Limitations in Chemistry

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## Abstract

The advancement in Artificial intelligence has ushered new opportunities in various aspects of life and fields of study. Among the various AI tools developed, chatGPT has gained considerable attention due to its natural language model and interactive capabilities. It has been recognized as a powerful tool for various applications in chemistry such as physical, organic, inorganic, analytical, industrial, environmental, polymer and food chemistry etc. in this review, we focused on the applications of chatGPT in the above named fields of chemistry. We discussed the evolution of chatGPT from the original GPT model to the current chatGPT model and we also examine the limitations of chatGPT. This review provides a comprehensive summary of the history, potential applications and limitations of chatGPT in the field of chemistry, along with in-depth insight on the future prospect of the technology.

**Keywords:** Artificial Intelligence; Chemistry, and Applications

## Introduction

As the world continues to evolve, technological advancements continue to evolve. The importance of technological advancement cannot be overemphasized. These technological advancements have a significant impact on the development and performance of language models, such as chatGPT. Different large language models have been developed with different applications and limitation in different fields [1]. Recently, the integration of Artificial intelligence in education has gained increasing attention particularly chatGPT. The recent technology Chat Generative Pre-trained Transformer (ChatGPT) is a free technology and can be accessible by the public. The trained model can answer follow-up questions, acknowledge its mistakes, limitations, incorrect premises, and reject inappropriate requests that may involve bridging ones privacy [2]. ChatGPT has gained a lot of attentions, hence many literatures has emerged

with researchers explaining the present and future trends. ChatGPT has brought a lot of controversy in the aspect of scientific writing, as most researchers are of the opinions that AI should be referenced as a co-authors Güzeldere and Franchi [3], the recent trends of AI particularly chatGPT is clearly reviewed in this paper, its history, application and limitations in chemistry. ChatGPT as an AI tool in chemistry helps in summarizing research papers, provide general experimental procedures, and compare experiment results, thus providing a more efficient approach than internet surfing.

## History

A.M. Turing, a computer scientist in 1950, explained the concept of whether machines can think and he demonstrated a famous test to determine whether humans can distinguish between conversations with humans and machines [4]. If the

interrogator cannot distinguish between the responses, the machine passes the Turing Test. The first chatbot created by MIT computer scientist Joseph Weizenbaum in the 1960s called ELIZA, passed the Turing test [5,6], arguably using certain tricks to pass the test [7] rather than exhibiting any significant intelligence. ChatGPT easily passes the Turing test, indicating that the era of AI has indeed arrived.

OpenAI's first large language model (LLM), called GPT-1, and was launched in 2017 followed by subsequent upgrades and different versions of GPT-2, GPT-3, and the widely-discussed chatGPT. ChatGPT is the recent trend. The technology was accessible for public use on November 30, 2022. ChatGPT's have had a significant growth rate which was 15 times faster than TikTok, one of the fastest-growing social media platforms [8]. Moreover, chatGPT has continued to set an unwavering record for growth, reaching 100 million users within two months of its launch [9].

## Applications

Despite being released to the public accessibility very recently, chatGPT has gained significant attention in chemistry and other related fields. One of the significantly anticipated applications of chatGPT is in the domain of education. AI and technology can be effective in education in several aspects, including personalized learning [10]. In this context, chatGPT has enhanced student participation, provide experiential learning, and help educators in the evaluation of exams and content preparation. Several researchers focused their studies on the impact of chatGPT in education because of its trend and various applications in the sector [11].

### Application of ChatGPT in Physical Chemistry

ChatGPT has various applications in physical chemistry and this include:

- Molecular modeling: chatGPT can be used to predict the behavior and structure of molecules based on quantum mechanics principles. This includes the prediction of energy levels, bond lengths, and vibrational frequencies.
- Reaction mechanism prediction: chatGPT can simulate chemical reactions and predict the outcomes in terms of reactant, product, and intermediates [12].
- Spectroscopy: chatGPT can be used to analyze spectroscopic data such as infrared, Raman and NMR spectra using machine learning algorithms. This will aid in identifying functional groups and the position of atoms in a molecule.
- Thermodynamic calculations: chatGPT can predict the properties of the system based on the measurement of physical properties such as pressure, temperature and entropy. It can also be used to measure thermodynamic parameters such as entropy, enthalpy, and Gibbs free

energy [13].

- Material design: chatGPT can be used to design new materials and predict their electronic and optical properties as well as mechanical characteristics [14].

### Applications of ChatGPT in Computational Chemistry

Also, in computational chemistry, chatGPT is used to generate human-readable explanations for complex chemical systems. For example, generating a detailed report on the properties of a molecule or the results of a simulation. This can greatly simplify the process of interpreting and communicating the results of computational chemistry studies [15]. ChatGPT can be used to generate predictions about the outcomes of different chemical reactions or to suggest new molecules that could be synthesized. This has helped computational chemists and other researchers to focus on more promising areas of research and this has helped to avoid wastage of resources and time on less promising research areas [16].

### Applications of ChatGPT in Analytical Chemistry

ChatGPT plays a significant role in accelerating analytical chemistry research by automating many tedious and time-consuming tasks, allowing researchers to focus on more crucial aspects of the research work and this can be applied in the field though:

Data analysis and interpretation: chatGPT can be used to analyze and interpret large data sets generated from analytical instruments. The model can learn the patterns in the data and provide insights into the chemical composition of the samples [17].

- Spectroscopy: chatGPT can be used to analyze spectroscopic data such as infrared, Raman and NMR spectra using machine learning algorithms. This will aid in identifying functional groups and the position of atoms in a molecule.
- Prediction of chemical properties: chatGPT can be used to predict the physical and chemical properties of molecules by training it on large databases of chemical structures and properties.
- Research article summarization: chatGPT can be used to summarize research papers in analytical chemistry, helping researchers to keep track of the latest developments in the field [18].

### Applications of ChatGPT in Environmental Chemistry

ChatGPT can be used in environmental chemistry to improve communication, collaboration, and knowledge

sharing among researchers, practitioners, and stakeholders. Here are some possible applications of chatGPT in this field:

- **Virtual event:** ChatGPT can be used as an alternative platform for organizing virtual event on environmental chemistry. Researchers from different parts of the world can join the chat room and share their findings, experiences, and insights without the need for onsite event. This will help in increasing the number of participant when compared to physical event [19].
- **Collaborative Teamwork:** With chatGPT, researchers can collaborate on research projects more effectively. They can use the chatbot to discuss research ideas, share data, and coordinate their efforts. This can help them to identify knowledge gaps, avoid duplicating efforts, and make more significant contributions to the field of environmental chemistry [20].
- **Science communication:** chatGPT can also be used to promote science communication among researchers and other stakeholders. This can help to bridge the gap between science and policy and increase public awareness and engagement in environmental issues [21].
- **Problem-solving:** chatGPT can also be used to solve environmental chemistry-related problems collaboratively. For example, a team of researchers who has worked on photocatalytic degradations of organic dyes can use the chat room to brainstorm solutions to treatment of waste water using photocatalysts and share ideas on the efficiency of the different catalyst each individual use for solving these issues [22].

### Application of ChatGPT in Organic Chemistry

Some of the potential applications of chatGPT in organic chemistry include:

- **Molecular design and reaction prediction:** chatGPT can predict the outcomes of chemical reactions by analyzing the reactants and their conditions. It can also suggest alternative reaction pathways or conditions that could lead to a higher yield or selectivity.
- **Nomenclature:** chatGPT can assist in naming organic molecules and compounds based on IUPAC standards. It can also suggest common names and provide explanations for their structures [23].
- **Data analysis:** ChatGPT can mine large sets of chemical data and identify patterns that could be useful in understanding structure-activity relationships. It can also perform regression analysis and predict physical and chemical properties based on molecular features [24].
- **ChatGPT as a tool in organic chemistry** has helped scientists generate new hypotheses, speed up the drug discovery process, and gain a deeper understanding of the field.

### Application of ChatGPT in Inorganic Chemistry

ChatGPT can analyze and summarize a vast amount of research works, articles, and publications on inorganic chemistry, enabling chemists to stay updated with the latest developments in their field. ChatGPT, has helped scientists to explore the huge Design-Space of chemical compounds and predict their properties and functionalities. This approach can also help in identifying potential catalysts and new materials that can be used in various applications [25]. **Predicting Reactivity and Mechanisms:** provides helpful insights into the likely reactions and reaction mechanisms for inorganic compounds **Virtual Screening of Drug Molecules:** It can predict drug-likeness, toxicity and pharmacokinetic parameters of these molecules, providing essential information to researchers on which compounds to focus on as potential drug candidates [26].

### Application of ChatGPT in Industrial Chemistry

ChatGPT can be applied in industrial chemistry as it can help to improve the efficiency, quality, and safety of manufacturing processes and they are vast applications of chatGPT in industrial chemistry, but are not only limited to; ChatGPT can be used to monitor the quality of products being manufactured in an industrial chemistry setting. By analyzing the data collected during the manufacturing process, ChatGPT can identify any issues that may be affecting the quality of the product and suggest ways to address these issues [27]. ChatGPT can identify any inefficiencies or bottlenecks in the process and suggest ways to optimize it. This can help to reduce costs and improve the overall efficiency of the process. ChatGPT can also be used to manage inventory in an industrial chemistry setting. By analyzing the data on the amount of raw materials and finished products, chatGPT can suggest the optimal inventory levels for the most efficient operation of the manufacturing process. ChatGPT can also be used to predict when equipment in an industrial chemistry setting may need maintenance.

In Research, ChatGPT can be used to generate abstracts, summaries, and even full research papers, written in natural language, which can greatly simplify the process of communicating research findings to a wider audience. This also includes writing summaries of sub-topics for a research work or reviews [28]. Other potential applications of chatGPT in chemistry include; providing quick and accurate answers to queries and summarizing results. Generating explanations for chemical structures, properties, characteristics of complex chemical reactions, and their mechanisms. Answering questions related to chemical concepts such as reactants, products, rate of reaction, theories, and principles. Predicting the thermodynamic properties of molecules and materials. Assisting with organic synthesis planning

and retrosynthetic analysis. Predicting chemical hazards, environmental effect, and toxicity of chemical substances. ChatGPT has vast applications in writing chemical equation, nomenclature, and chemical formulars [29].

### Limitations of ChatGPT

Although chatGPT as an AI tool has numerous applications in chemistry and may sound interesting and convincing, but don't take its word for it! Indeed, chatGPT's ability in forming meaningful and conversational sentences is quite impressive, but its responses in answering chemistry related questions needs to be verified. Recall, the field of chemistry deals with experiments and research and the chatGPT are programmed and as such, it's obvious it may 'hallucinate' responses from previous scientific articles and research [30]. Therefore, it is highly recommended to verify and fact-check any responses from chatGPT, because most responses may not be entirely correct. ChatGPT depends on pre-programmed data and it is limited [31]. When asked certain query beyond the programme in ChatGPT it gives responses such as "As an AI language model, I don't have the ability to perform certain functions".

### Question

Hi ChatGPT, draw the structure of glucose

### ChatGPT

I'm sorry, as an AI language model, I don't have the ability to draw images. However, I can describe the structure of glucose: Glucose is a monosaccharide and has the chemical formula  $C_6H_{12}O_6$ . It has a six-membered ring structure made up of five carbon atoms and one oxygen atom. Each carbon atom is bonded to a hydroxyl (-OH) group, except for one, which is bonded to a hydrogen (-H) atom. The remaining oxygen atom is also bonded to a hydroxyl group. The carbon atoms in glucose are numbered from 1 to 6, starting from the carbon atom bonded to the -H atom. Glucose is a polar molecule and can exist in two different forms - alpha-glucose and beta-glucose - depending on the orientation of the -OH group attached to the first carbon atom.

Furthermore, the current interface of chatGPT does not allow uploading of audio files or images. ChatGPT can produce code representations of visual images based on text prompts, but its drawing skills are somewhat limited currently. This is a limitation of chatGPT because early career chemists or beginners who are new to the field and may want to explore chatGPT in learning chemistry may experience difficulties in interpreting the code representation of visual images [31]. In this context, chemists experiences difficulties when solving issues in chemistry that involves putting structures in the

AI tool. No doubts chatGPT can write chemistry research abstract, summarize chemistry research papers, and answer chemistry related questions well enough to pass chemistry exams. Worryingly for students and research chemists is that students and scientists could deceitfully generate ideas as their own, or use such machine language to conduct an incomplete literature review and produce work that is unreliable thereby devaluing the field of study.

### Conclusion

"ChatGPT is here to stay". Although they are vast opinions on the implications and limitations of the technology, it is a powerful tool that is revolutionizing the educational sector including the fields of chemistry such assist ability to assist with literature searches, generate human-readable explanations for complex chemical systems, assist in the design and optimization of experiments, generate input files for computational chemistry software, predict properties of molecules and materials using quantum chemistry, and assist in the analysis of simulation data and the communication of research findings, opens a wide range of possibilities for this field. As AI continues to evolve and improve, researchers need to leverage on the powers of chatGPT and its exciting developments in the field of chemistry. One of the biggest limitations that chemists face is keeping up with the latest research in chemistry. With thousands of research papers published every day, it can be overwhelming to keep track of all the new findings. ChatGPT can help by generating relevant keyword-based queries and summarizing the results of literature reviews. This not only saves researchers time but also ensures that they do not miss any important studies that could be relevant to their work. ChatGPT has a vast limitation in providing citations and references. It is advisable to use chatGPT for basic instruction and simple task and not for complex queries.

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