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Review Article

Artificial Intelligence (AI) in the Chemical Field: Innovation and Risk Evaluation

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Keywords: AI – Artificial Intelligence; ML – Machine Learning; LLM – Large Language Models; Chat; Bot; Algorithm; Prompt; Chemistry; Chemicals; Errors; Hallucination; Risk; Precaution; Education; Research; Oncology

Abstract

This work aims to verify the various uses of AI in chemical settings and the benefits and risks of using this innovative technology.

AI tools make it possible to have a powerful instrument in study or research, as well as in various chemical disciplines.

After a review of some interesting scientific literature related to some interesting uses of AI and the risks involved, the results of an experimental project involved the use of a famous free AI CHATBOT (question and answer).

The articles reported are involved with some benefits of AI use, but also related to the specific risks.

Crucial in this world is that the results provided must be the right ones, without relevant error or the so-called "hallucinations".

The results of a specific experimental project using a free AI chatbot show errors in providing one.

Chemical structure: The final human control of the AI results can be a useful method to use in a safe way for this technology today.

Introduction

AI and ML instruments are widely introduced in many sciences and also in chemistry settings: the use can be from predicting chemical properties, rational design of new molecules, automated systems planning, material design, retrosynthetic analysis, spectroscopy technique, separation technique, chemoinformatics, proteomics, drug research, chemistry learning, and many other areas.

Of interest to observe what is happening in various chemical disciplines: opportunities and risks.

According to how are chatbots transforming the oil and gas industry:

Abhishek Shanbhag, November 8, 2021: "Oil and gas companies are exploring new ways to leverage AI to automate and digitize processes, increase productivity, and solve complex and straightforward engineering challenges."

Innovation Science

How AI Can Help Find New Minerals on Earth and Other Planets

ByDavid Bressan, Senior Contributor. David Bressan is a geologist who covers curiosities about Earth.

Jun 19, 2023

"Given the basic mineral composition of the Tecopa

formation, the AI was able to predict the locations of exotic uranium minerals (like rutherfordine, andersonite, schröckingerite, bayleyite, zippeite). The model located promising areas for critical rare earth elements and lithium minerals (including monazite, allanite, and spodumene)."

Smart Automation in Metallurgy: How AI Is Revolutionizing the Metallurgical Industry

Richardson Cau

08-04-2025

Iconic Research and Engineering Journals

"The metallurgical industry has historically relied on heavy machinery, manual labor, and conventional process optimization techniques. With the advent of AI, the sector is undergoing an unprecedented transformation. This work explores the integration of AI-driven smart automation in metallurgy, examining its impact on efficiency, sustainability, and economic viability. AI algorithms enhance predictive maintenance, defect detection, and quality control, reducing material waste and operational downtime. ML models improve alloy composition prediction and process parameters, ensuring greater consistency and performance in metallurgical applications. The incorporation of AI-driven robotics minimizes human exposure to hazardous environments, increasing workplace safety."

In the context of AI chatbots, a prompt is a user-provided instruction or question that guides the AI's response.

The chatbot algorithm learns the data from past conversations and understands the user's intent.

A prompt for an AI chatbot is a piece of text that serves as an instruction or question given to the AI to guide its response.

ML makes AI training possible.

Chatbots can use both AI and ML tools, and they are conversational-based.

Generative AI is revolutionizing chemistry by accelerating drug discovery, optimizing material design, and streamlining research processes. (Design of new molecules, predicts properties, automated tasks, and many other tasks).

Versus the classic Browser, the AI chatbot provides a unique response instead of the browser providing multiple responses from various sources (the user cha verify the goodness of this website).

Today, the most recent version of some famous chatbots can show about 88,7% in scores of accuracy.

Review Clin Lab Med. 2023 Mar; doi: 10.1016/j.cll.2022.09.005.

Artificial Intelligence Applications in Clinical Chemistry Dustin R Bunch, Thomas J.S. Durant, Joseph W Rudolf

"AI applications are an area of active investigation in clinical chemistry. Many publications have demonstrated the promise of AI across all phases of testing, including preanalytic, analytic, and postanalytic phases; this includes novel methods for detecting common specimen collection errors, predicting laboratory results and diagnoses, and enhancing autoverification workflows. Although AI applications pose many ethical and operational challenges, these technologies are expected to transform the practice of the clinical chemistry laboratory shortly."

Dr Kevin Jablonka

"Incorrect answers with high conviction can lead to problems."

"This was particularly noticeable with questions on the interpretation of chemical structures, like as the prediction of NMR spectra". The models seemed to provide clear answers, even if they sometimes made fundamental errors. The human experts hesitated more often and questioned their conclusions. "This discrepancy is a decisive factor for the practical applicability of AI in chemistry," because "A model that provides incorrect answers with high conviction can lead to problems in sensitive areas of the research."

Harnessing AI for Geosciences Education: A Deep Dive into ChatGPT's Impact

Subham Patra, T. Sumit Singha, Megh Kanvinde, Angana Mazumdar, and Swastika Kanjilal- Preprint

"The survey findings reveal that ChatGPT is gaining popularity among geoscience students, with many using it as a quick information retrieval tool and for content generation tasks. Students expressed concerns about its level of accuracy, potential biases, and lack of awareness regarding its limitations. While ChatGPT offers benefits in terms of generating content and streamlining educational tasks, it cannot replace the essential role of human teachers in fostering critical thinking and problem-solving skills."

Alan Johnson

22 novembre 2024

"In the rapidly evolving field of chemical regulatory compliance, AI has emerged as a kind of transformative force. For companies operating across multiple jurisdictions, navigating the labyrinth of global regulations—each with its nuances, updates, and enforcement trends—is increasingly unmanageable without leveraging cutting-edge technology. AI has not only streamlined this complexity but has also unlocked new possibilities for proactive compliance strategies."

Between Truth and Hallucinations: Evaluation of the

Performance of Large Language Model-Based AI Plugins in Website Quality Analysis

by Karol Król

Appl. Sci. 2025, https://doi.org/10.3390/app15052292

"The general conclusion is that using AI tools without considering their characteristics may lead to the propagation of AI hallucinations in audit reports."

AI Ethics. 2024 May 27; doi: 10.1007/s43681-024-00493-8

The ethics of using artificial intelligence in scientific research: new guidance needed for a new tool

David B Resnik, Mohammad Hosseini

"AI systems can make systemic and random errors."

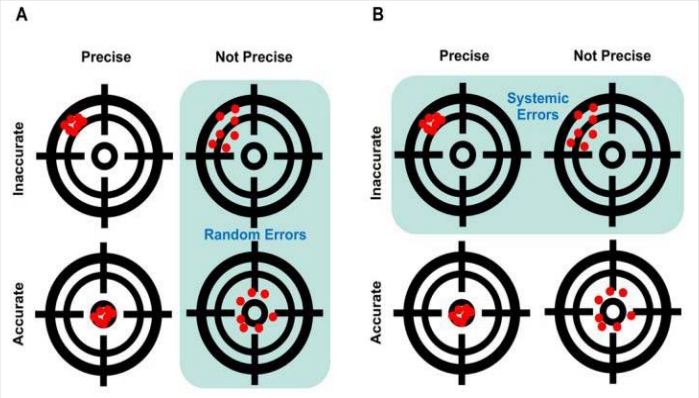


Figure 1: Random errors *vs.* systematic errors. From doi: 10.1007/s43681-024-00493-8.

AI Soc. 2022 Nov 17:1–24.

Omission and commission errors underlying AI failures

Sasanka Sekhar Chanda, Debarag Narayan Banerjee

"AI systems can fail (a) if there are problems with its inputs comprising various representations of data, sensor hardware, et other and/or (b) if the processing logic is deficient in some way and/or (c) if the repertoire of actions available to the AI system is inadequate, in ex. If the output is inappropriate. These problems/deficiencies/inadequacies originate from two kinds of errors—commission and omission errors —in the design, development, and deployment of an AI system. These errors are defined:

Error of commission: doing something that should not have been done.

Error of omission: not doing something that should have been done."

Science chatbots provide a unique way to interact with complex scientific topics, giving users instant answers, guidance, and useful support. These AI instruments have been developed to simplify the study of science, covering subjects from biology and chemistry to physics and beyond.

06 February 2024

AI chatbot shows surprising talent for predicting chemical properties and reactions.

Researchers lightly tweak ChatGPT-like system to offer chemistry insight.

By Davide Castelvecchi

"With only a little fine-tuning, a machine-learning system similar to ChatGPT can become surprisingly adept at answering research questions in the chemistry field. When predicting the properties of molecules and materials or the yields of reactions, the general-purpose system can match or beat the performance of more specialized models while requiring a smaller amount of tweaking, researchers write today in Nature Machine Intelligence."

Material and methods

With an observational point of view, relevant literature (from 1 to 9) related to the topic is reported.

All literature comes from a scientific database

Various Figures 1,2 help in the general meaning

After these phases, an experimental project is submitted to test a famous AI chatbot and report the response to the questions.

After all this, and conclusion is provided to the researcher.

Results

From literature

Kassem Hallal, et al.

"Molecular Formula: ChatGPT gave the DU values with 90% correctness in trial one and 80% in trial two. The comparison between the correct answers in both trials revealed only a 70% match. Bard poorly answered this question with 20% correctness in T-1 and 24% in T-2, but there was an 83% match in correct answers between both these trials" [1].

Giacomo Rossettini, et al.

"AI chatbots' accuracy

Overall, we found a statistically significant difference in accuracy between the answers of the three chatbots ($p < 0.001$)."

"Although AI chatbots showed a promising accuracy in predicting the correct answer in the Italian entrance university standardized examination test, we encourage candidates to

cautiously incorporate this new technology to supplement their learning rather than as a primary resource."

Related accuracy of some AI tools in entrance test in degree course: "We encourage candidates to cautiously incorporate this new technology to supplement their learning rather than a kind of primary resource" [2].

J Chem Inf Model. 2025 Apr 22; doi: 10.1021/acs.jcim.4c02322

Augmented and Programmatically Optimized LLM Prompts Reduce Chemical Hallucinations

Scott M Reed

"As LLMs and their training data grow in size, their capabilities can seem limitless; they cannot be trained on data that does not exist yet. The approach described takes an LLM incapable of a specific molecular task and makes it substantially more capable through augmented generation and prompt optimization" [3].

Michele Salvagno, et al.

"AI chatbot and ChatGPT in particular appear to be useful tools in scientific writing, assisting researchers and scientists in organizing material, generating an initial draft, and/or proofreading. There is no publication in the field of critical care medicine CCM prepared using this approach; this will be a possibility shortly. ChatGPT work should not be used as a replacement for human judgment and the output should always be reviewed by experts before being used in any critical decision-making. Many ethical issues arise about using these tools, such as the risk of plagiarism and inaccuracies, as well as a potential imbalance in its accessibility between high- and low-income countries, if the software becomes paying" [4].

He S Yang, et al.

"Chatbots, which are rapidly evolving AI applications, hold tremendous potential to improve medical education ME, provide timely responses to clinical inquiries concerning laboratory tests, assist in interpreting laboratory results, and facilitate communication among patients, physicians, and laboratorians. Users should be vigilant of existing chatbots' limitations, such as misinformation, inconsistencies, and a lack of human-like HL reasoning abilities. To be effectively used in laboratory medicine, chatbots must undergo extensive training on rigorously validated medical knowledge and be thoroughly evaluated against standard clinical practice" [5].

JD Mendez

"This study highlights the need for training on responsible AI use to address ongoing ethical concerns over the misuse of these systems and to get ahead of future issues" [6].

Tathagata Pradhan, et al.

"The Future of ChatGPT in Medicinal Chemistry MC envisions AI-driven breakthroughs in drug discovery DD. Utilizing advanced language models like ChatGPT accelerates screening and optimization of chemical compounds, predicting their interactions and properties. This synergy of AI and Medicinal Chemistry MC promises to revolutionize pharmaceutical research" [7].

AJay Vikram Singh, et al.

"Chemical risk assessment plays a pivotal role in safeguarding public health PH and environmental safety ES by evaluating the potential hazards and risks associated with chemical exposures. In recent years, the convergence of AI, ML, and omics technologies has revolutionized the field of chemical risk assessment CRA, offering new insights into toxicity mechanisms, predictive modeling, and risk management strategies" [8].

Experimental part

1) Example of a question submitted to a famous AI-CHAT BOT of free access:What is the chemical formula of titanium dioxide? Response provided: Ti02

2) What is the PH of a chloric acid solution 0,1 molar? Response PH=1

3) What is the water solubility of calcium chloride at 20 °C? Response received 74,5g/ 100 ml of water

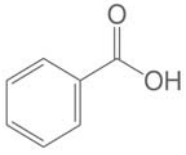
4) What is the pure water conductivity? responce around 0,055microsiemens per cm

5) What is the boiling point of exane? Response approximately 68,7 centigrades

How many carbon atoms are there? 5 atoms (2 from the aldehyde group and 3 from the three CH2 groups

6) Write the first principle of thermodynamics: response DELTA U = Q-L, where DELTA U is the internal energy variation of the system, Q heat absorbed by the system, and L is = work done by the system on the environment

7) Write the chemical structure of benzoic acid: response received



8) What is the composition of medium carbon steel: response carbon content ranging from 0,30% to 0,60% by weight (Mn 0,60% - 1,65%, P < <= 0,040%, S <= 0,050%, Iron 98-99%)

9) Write the balanced reaction of sodium hydroxide plus sulfuric acid: response

H_2SO_4 + 2 NAOH ------ → NA_2SO_4 + 2 H_2O

10) Is the activated charcoal a crystalline substance? Response no, it is amorphous

11) How is the conductivity of copper? Response 5,96 x 10^7 S/m siemens per meter at room temperature

12) What is the electronic configuration of chlorine? At number 17

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^5$

13) What can be the nuclear radiation? Response: alfa, beta, gamma, and neutron (added question: and the x-ray? New response, these are not nuclear radiation but a type of electromagnetic radiation generated outside the nucleus

14) How much oxygen can be released by an oxygen medical cylinder with 3 3-liter volume at 200 atm: response 600 liters. P1*V1 P2*V2 Boyle's law: 200*3= 1 V2

15) Write the chemical structure formula of polivinyl chloride:

$[-CH_2–CHCl-]_n$

16) What is the crystalline status of diamond? Response Cubic (also known as isometric)

17) What components are present in an MS GAS chromatograph-mass spectrometer? Response GC component: carrier gas supply, injector GC column, oven (that maintains and controls the temperature of the column), interface between GC and MS (Transfer line) and MS component ion source, mass analyzer, detector, vacuum system, and computer software.

18) The UV ultraviolet radiation region, what wavelengths include ?: response from 10 to 400 nanometers

19) What types of chromatographic columns are there? responce

Based on technique: GAS chromatography, capillary columns, packed columns, LC liquid chromatography

HPLC, ULTRA HPLC

Based on the separation principle: reverse phase, normal phase, ion exchange, size exclusion, affinity column

Specialized column: chiral column, monolithic column, capillary electroforesis

20) How is dynamite produced? It is a high explosive invented by A.Nobel in 1867. It is made by safely stabilizing nitroglycerin, which is a very sensitive and powerful liquid explosive, by absorbing it into an inert material. (Mixing nitrolycerin with Kieselguhr, a type of diatomaceous earth and stabilizes it).

The dynamite paste is packed into paraffin-coated paper tubes (about 20 cm x 3,2 cm).

21) What light is emitted by lithium when heated? It emits light in the red region of the visible spectrum: the most prominent mission line is at 670,8 nm, which is a deep red color. (Lithium salts produce a crimson or carmine-red flame in flame tests).

22) How are borosilicate glasses? By melting and refining a mixture of raw materials at high temperature, followed by forming and annealing processes. It is known for its excellent thermal and chemical resistance and is widely used in laboratory glassware (the raw materials used are: silica, boron oxide, soda, alumina, lime, other oxides; typical composition about 70-80 Sio_2,10-15% B_2O_3, 2-3 % Al_2O_3, less than 5% alkali and alkaline earth).

23) What is the fractioned distillation process in petroleum products production? It is a crucial process used in the petroleum industry to separate crude oil into different components of fractions based on their boiling points.

24) Each fraction corresponds to a group of hydrocarbons with similar molecular size and physical properties, to produce gasoline, diesel, kerosene, naphta, and lubricating oil.

25) What principles are used in a mass spectrometer? are used chemico phisical principles to detect and analyze molecules based on their mass-to-charge ratio (m/z): ionization to be manipulated by electric and magnetic fields, mass to charge separation using electric or magnetic fields (to separate for the identification of different ions in a mixture). Detection measures the signal produced. Data interpretation.

26) What is the fingerprinting zone in spectroscopy? It is a part of the IR spectrum (about 1500 to 500 CM-1 that contains a complex set of absorption bands unique to individual molecules. This helps confirm the identity of a compound, even for isomers or compounds with a similar structure.

It is unique because this region contains numerous bending and skeletal vibrations of the molecule.

This vibration involves complex motion of the molecule's entire framework and is highly sensitive to small changes in molecular structure. (For example, ethanol and methanol may have similar -OH group stretches around 3300 cm^{-1}, but their fingerprint region will differ, allowing them to be distinguished).

27) Describe the Rutherford experiment for the atom structure theory: The Rutherford experiment, also known as the gold foil experiment, was a groundbreaking experiment in atomic physics conducted in 1909 by Hans Geiger and Ernest Marsden under the supervision of Ernest Rutherford. This experiment led to a major revision of the atomic model.

A thin sheet of gold foil (only a few atoms thick) was bombarded with alpha particles (positively charged particles emitted from radioactive materials).

Around the foil, a fluorescent screen coated with zinc sulfide was placed to detect the scattering of the alpha particles. Tiny flashes of light would appear wherever an alpha particle struck the screen.

At the time, J.J. Thomson's "plum pudding model" was widely accepted. It suggested:

Atoms are made of a diffuse cloud of positive charge.

Electrons are embedded within this cloud, like raisins in pudding.

Prediction: Alpha particles should pass through the atom with minimal deflection, as the positive charge was thought to be spread out evenly.

Actual Observations

Most alpha particles passed straight through the foil with no deflection.

Some particles were deflected at small angles.

A few particles (about 1 in 8,000) were deflected back at large angles, even close to 180 degrees.

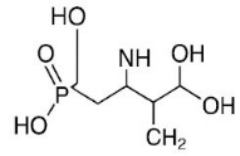
Rutherford concluded that:

Most of the atom is space, allowing most particles to pass through.

There is a dense, positively charged core (later called the nucleus) that repelled some alpha particles.

Electrons orbit this nucleus at a distance, like planets around the sun.

28) Write the Glifosate structure formula: result provided



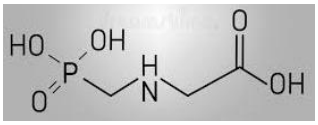


Figure 2: The right glyphosate structure formula (There is a -COOH group on the right)

Results of the tests: on 28 questions submitted (topic chemistry) to the chatbot, 27 were correct and 1 not incorrect.

3,57% of responses were wrong (so 96,43% are to be considered right).

The wrong response was involved in the writing of a chemical structure formula.

Discussion

Observing the international scientific literature, it is possible to verify that there is a double face of the AI–CHAT BOT instruments in scientific disciplines like chemistry: great efficacy in producing responses to the various questions submitted, but also a profile of error and a % of mistakes not irrelevant.

In our experiment, about all 28 questions in the chemistry field 27 were provided by the chatbot in the right way.

The 28th question to the chatbot presents a formula different from the right one.

(These results come from using a free version of a famous chatbot available on the web).

Probably, if a new test the question related chemical structure formulas are a greater number, more than 1, the possibility of error can increase.

This kind of error is relevant because in chemistry, the exact chemical formula is fundamental to predicting reactions (functional groups and other chemical and physical properties).

Of this, the scientific community must take in the right consideration to avoid accidents in the chemistry lab or during the synthesis, or other chemical transformation or reaction.

Chemistry is not a scientific discipline based on absolute certainty, but based on observation and on experimental process, study of the models and their transformation, and this requires high accuracy.

Other implication: at what level is it ethical to use an AI catbot to write a university thesis and research?

And this use will produce in the next years a more weak brain in students or researchers due to a reduction of the intellectual efforts to reach the solutions managing the chemical problems?

Conclusion

In order to get the best results possible from a chatbot, it is necessary to verify the kind of version because not all versions can provide an equal level of accuracy in response (see the various providers and the free or professional providers).

Rules in the chat research to be efficacy: BE SPECIFIC, USE CLEAR INSTRUCTIONS, BREAK DOWN COMPLEX REQUESTS, PROVIDE THE RIGHT CONTEXT, MAKE FOLLOW-UP QUESTIONS to better focus.

In the experiment submitted in this work, the results of

3,57% of error are a significant level to be taken in the right consideration.

Even if the majority of responses obtained can be useful for chemistry students or professionals, it must be taken into consideration that the risk of errors or hallucination, or other problems linked to the actual status of the version used. (Probably in the future, this accuracy will be improved).

Other problems are: the capacity to submit all the sources used by the chatbot, the database used can be obsolete, the efficacy of the prompt chosen, insufficient time for training with the data available, contextual ambiguity problems, the language model used, misinterpretation of the input, and emerging topics.

(Few data available today), overconfidence, contextual gaps, overgeneralization, and ethical implications.

The accuracy of the chatbot depends on the providers (not all are equal).

Of interest is to use of the chatbot science science-focused use (chemistry).

As a final consideration by the author: in the chemistry field (but also in other disciplines like toxicology or oncology and other related fields), the AI chatbot used in this work, even if of great utility not provide a highly accurate response to all chemistry questions as requested by this scientific discipline.

In future studies, it will be mandatory to verify the accuracy of the questions submitted to the AI chatbot of more advanced generations because more efficient than the free version.

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