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AI ARTIFICIAL INTELLIGENCE IN CHEMICAL FIELD – INNOVATION AND RISK EVALUATION

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Abstract: Aim of this work is to verify the various use of AI in chemical settings and the benefit and risk in using this innovative technology. AI tools like make possible to have powerful instrument in study or in researcher as well as in the various chemical discipline. After a review of some interesting literature related some interesting use of AI and the risks involved the results of an experimental project involved the use of a famous free AI – CHATBOT (question and answer). Crucial in this world is that the results provided must to be the right one , without relevant error or the so called "hallucinations". The final human control of the AI results can be an useful method to use in a safety way this technology today.

Keywords: AI – artificial intellience ,ML machine learning, LLM large Language models, chat- bot, algorytm Prompt , chemistry, chemicals,Errors, hallucination , risk, precaution , education , research, oncology.

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INTRODUCTION

AI and ML intruments are wi dely introduced in many sciences and also in chemistry settings:the use can be from Predictin chemical properties, rational design of new molecules ,automated systesys planning, materiald design, retrosysntesys , spettroscopy technique , separation technique , chemioinformatics, proteomics , drugs research, chemistry learnig and many other. Of interest to observe what is happening in various chemical discipline: opportunity and risks.

According 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

By David 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 element 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 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 possible AI training

Chat bot 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).

Versus the classic Browser the AI chat bot provide a unique responce insted the brower provide different multiple repsonce form various source (the user cha verify the goodness of this web site).

Today the most recent version of some famous chat- bot can show about 88, 7% in scores of accurancy.

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

Artificial Intelligence Applications in Clinical Chemistry Dustin R Bunch, Thomas Js 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, or 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 in the near future."

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 own 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 the 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 the 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 the 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 a 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 the 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"

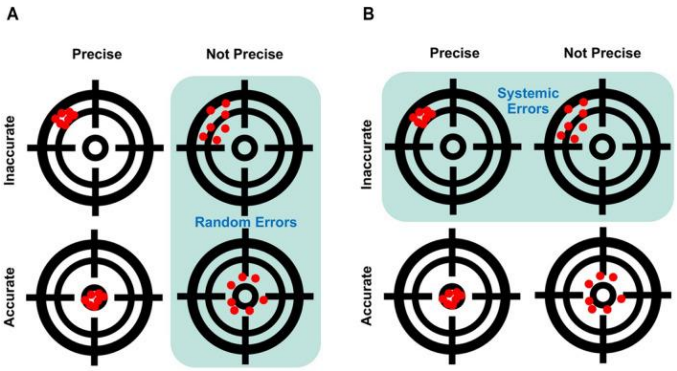


Fig n 1 Random errors vs systematic errors .From doi: 10.1007/s43681-024-00493-8

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

Science chatbots provide a unique way to interact with the complex scientific topics, giving users instant answers, guidance, and useful

support. These AI instruments have been developed to simplify the study of the 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 chemistry field. When predicting the properties of the 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

Whit and observational point of view relevant literature related the topic is reported.

All literature comes from scientific database

Various figures(1-2) helps in the general meaning

After this phases and experimental project is submitted to test an famous AI chat -bot end reported the response to the questions.

After all this and final 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 83% match in correct answers between both this 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 an primary resource."

Related accurancy 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 the scientific writing, assisting researchers and scientists in organizing material, generating an initial draft and/or in proofreading. There is no publication in the field of critical care medicine CCM prepared using this approach; this will be a possibility in the next future. 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 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)

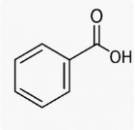
Ajay Vikram Singh et al

"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

Example of question submitted to a famous AI-CHAT BOT of free access:

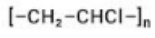
- What is the chemical formula of titanium bioxide ? reponce provided : Ti02
- Waht is th PH of an cloridric acid solution 0,1 molar? Responce PH=1
- What is the water solubility of calcium chloride at 20 grades? Responce received 74,5g/ 100 ml of water
- What si the pure water conducibility ? responce around 0,055microsiemens per cm
- What is the boiling point of exane ? responce approximatively 68,7 centigrades
- How many carbon atom have glutaraldeide ? 5 atoms (2 from the aldeides group and 3 from three ch2 groups
- Write the first principle of thermodinamycs : responce DELTA U = Q-L where DELTA U is the internal energy variation of the system, Q= heat absorbed by the system and L = work done by the system to the environment
- Write the chemical structure of benzoic acid : responce received



- What is the composition of medium carbon steel : responce carbon content rangin from 0,30% to 0,60% by weight (Mn 0,60% - 1,65%, P < or = 0,040%, S <or = 0,050%, Iron 98-99%)
- Write the balnced rection of sodium idroxide plus solforic acid: responce
- H2SO4 + 2 NAOH ------→ NA2SO4 + 2 H2O
- The activted charcoal is a cristalline substantia? Responce no , it is amorphous
- How is the conductivty of copper?response 5,96 x10^7 S/m siemens per meter at room temperature
- What is the electronic configuration of clorine? At number 17

- What can be the nuclear radiation? Responce : alfa, beta, gamma and neutron (added question : and the x-ray ? new responce this are not nuclear radiation but a type of electromanetic radiation generated outside the nucleus
- How much oxigen can be relased by an oxigen medical cylinders 3 liter volume at 200 atm : responce 600 liter P1*V1= P2*V2 Boyle law 200*3= 1 V2

Write the chemical structure formula of poli vinil clorure :



- Waht is the cristalline status of diamond? Responce Cubic (also known as isometric)
- Waht component are present in a MS GAS mass spectrofotometer? response GC component : carrier gas sypply, injector GC colum, oven (that mantein and contro, the temperature of the colum), interface between GC and MS(Transfer line) , and MS component ion source, massa analyzer ,detector, vacum system, computer software.
- The UV ultraviolect radiation region what wavelengts include ?: responce from 10 to 400 nanometers
- What type of chromatographic colum there are ? response.
- Based on technique: GAS chromatography, capillary colums, paked colums,LC liquid chromatography

HPLC, ULTRA HPLC

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

Specialized column: chiral colum, monolithic colum, capillary electroforesis

- How is produced dynamite? It is an high explosive invented by A.Nobel in 1867 , it is made by safely stabilizing nitrolycerin , whic 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).

- What ligh is emitted by litium when heated ? it emitts light in the red region of the visible spectrum : the most prominente mission line is at 670,8nm which is a deep red color.(lithium salts produce a crimson or carmine - red flame in flame tests).
- How are produced borosilicate glasses? By melting and refining a mixture of raw materils at high temperature, followed by fornming and annealing prpcesses. It is know for its excellent thermal and chemical resistance and widely used in laboratory glassware (the raw materia used are : silica, boron oxide, soda,alumina,lime other oxidex ; typical composition about 70-80 Sio2 ,10-15% B2O3, 2-3 % Al2O3, less then 5% alkali and alkaline earth).
- What is the fractioned distillation process in petroleum products production? it isa crucial process used in the petroleum industry to separate crude oil into different components of fractions bassed on their boiling points .
- Each fraction correspond to a roup of hydrocarbons with similare molecular size and physical properties, to produce gasoline, diesel, kerosene , naphta and lubricating oil.
- What principle is used in mass spectrometer? are used chemico phisical principles to detect and analysis of molecule based on theirmass-to -charge ratio (m/z): ionization to be manipulated by electric and manetic field,mass to charge separation using electric or manetic fields (to separate for the identification of differen ions ina a mixture). Detection measuring ions signal produced. Data interpretation.
- What is the fingerprinting zone in spettrosvcopy ? : it is a part of IR spectrum (about 1500 to 500 CM-1 that contain a complex set of absortion bands unique to individual melocules. This helps confirm the identity of a compound, even for isomer or compounds with similar structure.

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

These vibrations involve complex motion of the molecule entire framework and are highly sensitive to small changes in molecular structure. (in example ethanol and methanol may have similar -OH group streches around 3300 cm-1 but their fingerprint region will differ , allowing them to be distinguised.)

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.

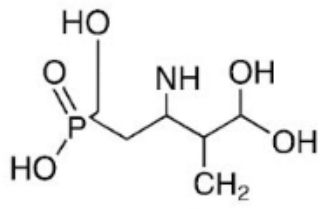
Rutherford concluded that:

Most of the atom is empty 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.

Write the Glifosate structure formula: result provided



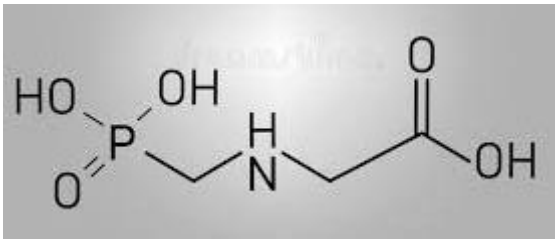


Fig n 2 the right Gifosate structure formula (There is a -COOH group on the right)

Results of the tests: on 28 question submitted (topic chemistry) to the chat – bot 27 was right and 1 not correct.

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

The wrong responce was involved in the writing of an 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 discipline like chemistry: great efficacy in producing responce to the various question submitted but also an profile of error and a % of mistake not irrilevant.

In our experiment about the all 28 question in chemistry field 27 was provided by the chat bot in right way

The n. 28 question to the chat- bot present a formula different form the right.

(This reults come from using a free version of a famous chat bot available on web.)

Probably if a new test the question related chemical structure formula is a gretar number more then 1 the possibility of error can increase).

These kinds of error are relevant because in chemistry the exact chemical formula is fundamental to predict reaction (functional groups and other chemical physical properties).

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

Chemistry is not a scientific discipline based on absolute cernainty but based on the observation and on experimental process, study of the modesl and its transformation and to do this require high accurancy.

Other implication: since what level is ethical to use AI cat-bot to write university thesis and research?

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

CONCLUSION

In order to get the best results possible form a chat-bot it is necessary to verify the kind of version because not all version can provide equal level of accurancy in responce (see the various provider and the free or professional provider) .

Rules in the chat research to be efficacy: BE SPECIFIC, TO BE USED CLEAR INSTRUCTION, BREAK DOWN COMPLEX REQUEST, PROVIDE THE RIGHE CONTEXT, and MAKE FOLLOW UP QUESTION in order to better focus.

In the experiment submitted in this work the results of 3, 57% of error is a significative level to be taken in the right consideration.

Even if the majority of responce obtained can be useful for chemistry students or professionals it must to be take in consideration the risk of errors or hallucination or other problem linked to the actual status of the version used .(probably in future this accurancy will be improved) .

Other problem are : the capacity to submitt all the source used by the chat -bot: the databese used can be obsolete) , the efficacy of the prompt choosed, insufficient time for trainind by the data available, contextual ambiguity problems , language model used, misinterpretation of the imput , emerging topics

(Few data available at today), overconfidence, contestual gaps,overgeneralization, ethical implication.

The accurancy of the chat bot depends by the providers (not all are equal) .

Of interest to use the chat bot science focused. (chemistry)

As final consideration by the author : in chemistry field (but also in other discipline like toxicology or oncology and other linked) the AI chat bot used in this work even if of great utility not provide really high accurate responce to all chemistry question as request instead by this scientific dicispline.

CONFLICT OF INTEREST: no

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