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Enhancing catalysis studies with chat generative pre-trained transformer (ChatGPT): Conversation with ChatGPT†

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The progress made in natural language processing (NLP) and large language models (LLMs), such as generative pre-trained transformers, (GPT) has provided exciting opportunities for enhancing research across various fields. Within the realm of catalysis studies, GPT-driven models present valuable support in expediting the exploration and comprehension of catalytic processes. This research underscores the significance of ChatGPT in catalysis research, emphasizing its prowess as a valuable tool for furthering scientific inquiries. It suggests that for an outstanding oxygen evolution reaction (OER) catalyst as a case study, scientists can leverage ChatGPT to extract deeper insights and brainstorm innovative approaches to grasp the mechanism better and refine current systems.

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Introduction

The human species, *Homo sapiens*, has long been recognized as the most intelligent life form on Earth, possessing large brains that provide significant cognitive abilities and processing capacity, surpassing those of all other species.¹ Over millions of years of evolution, humans have experienced remarkable growth in brain size and intelligence, setting them apart from other organisms in terms of intellectual capabilities. Our intelligence has always played a pivotal role in our identity and pursuits. For countless generations, we have strived to comprehend the inner workings of our minds and behaviors, and the human brain, a marvelously intricate organ consisting of mere matter, can perceive, grasp, predict, and manipulate a world that surpasses its scale and complexity.² It is this profound exploration that has given rise to the field of artificial intelligence (AI), which seeks not only to comprehend but also to create intelligent entities or machines capable of deciphering effective and secure courses of action across a vast array of novel circumstances. Recently, significant advancements have been made in natural language processing (NLP),

enabling its successful application in various real-world scenarios such as speech and entity recognition, summarization, language translation, and text generation.^{3–5} Researchers have extensively utilized recurrent neural network (RNN) models in many of these applications, leveraging their recurrent structure to capture dependencies within texts.^{3–5} However, RNN models have limitations in handling long-range dependencies present in natural language texts.⁴ To address this issue, a transformer architecture was introduced.^{6–9} A transformer is an autoregressive, self-supervised language model that incorporates a self-attention mechanism to effectively determine the relationships and relevance among different parts of inputs. This self-attention mechanism enables the model to robustly understand the relationship between words in a sentence, independent of their position.^{6–9}

Generative pre-trained transformer (GPT)-3, based on the transformer architecture,^{7,8} is a large language model (LLM) that has achieved remarkable success in various NLP tasks. GPT-3 is trained on a vast amount of text data, containing around 175 billion trainable parameters and approximately 570 GB of text. As a result, and interestingly, it is able to generate human-like text and perform language-related tasks with high accuracy.

ChatGPT, developed by OpenAI,¹⁰ is an NLP model that was launched in November 2022.⁹ It represents a breakthrough in LLMs as it can generate text while maintaining a conversational style that closely resembles human conversation. Although ChatGPT shares its foundation with GPT-3, it addresses the issue of “poorly characterized behavior” associated with GPT-3.¹¹ To mitigate the generation of toxic or untruthful outputs, ChatGPT employs three different strat-

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egies: supervised fine-tuning, reward modeling, and reinforcement learning. The process starts by collecting a dataset of labeled demonstrations, which is then used to fine-tune GPT-3 through supervised learning. Subsequently, a dataset of rankings for model outputs is employed to further enhance the model using reinforcement learning with human feedback. The resultant model, known as InstructGPT,¹¹ exhibits improved behavior and produces more reliable and contextually appropriate responses. In contrast to other AI-based language models, ChatGPT generates entirely new content in real-time conversations, catering to user queries and maintaining a consistent and engaging dialogue style. This attribute sets ChatGPT apart from other LLMs, making it a more unique and versatile model.

ChatGPT has demonstrated exceptional performance across various application domains, including coherent content and essay generation, chatbot responses, language translation, question answering, and even programming code.^{12,13} Ongoing research aims to fine-tune LLMs like ChatGPT for specific tasks and explore transfer learning in new domains. In an educational context, ChatGPT can be highly beneficial for both students and educators. Educators can leverage ChatGPT to prepare course outlines, develop topic-related content for lectures and presentations, generate questions and problem sets, and more. Similarly, students can utilize ChatGPT to solve complex problems, seek explanations for specific topics, draft essays, and receive programming-related support, thereby accelerating their learning process.^{13,14}

While ChatGPT has made considerable progress, concerns regarding its misuse have also been raised.^{15–17} Thus, it is crucial to carefully consider potential threats such as the integrity of online exams and question answering, alongside the numerous positive applications of ChatGPT in education. Experts have expressed apprehension about the impact of ChatGPT on common practices like programming.¹⁶ Therefore, it is essential to evaluate the situation rationally and develop suitable educational plans in light of evolving technologies such as ChatGPT. In recent decades, several technologies have emerged that have disrupted traditional practices, prompting individuals to evaluate the benefits and risks associated with these innovations.¹³ Similar questions have been raised about the impact of Google on cognition, reading, and memorization.¹⁸ Massive open online courses (MOOCs) also attracted significant attention in the early 2010s but experienced a decline due to issues with their strategies and business models.¹⁹ Similarly, ChatGPT not only holds immense potential but also raises a significant concern.

Shortly after the introduction of ChatGPT, many scientists in various fields realized its revolutionary benefits in various stages of their research. From aiding developers in debugging and code analysis²⁰ to providing a scaffold for informed decision-making in public health,²¹ its capabilities seem to stretch across diverse domains. In agriculture, it hints at a future where data analysis provided by models like ChatGPT can inform crop forecasting and pest manage-

ment.²² In additive manufacturing (AM), multiple studies underscore ChatGPT's capability in enhancing the end-to-end workflow from design conception to manufacturing execution. Notably, these models exhibit proficiency in intricate tasks like converting text prompts to design specifications and optimized G-code generation for specific materials and objects in 3D printing, for dealing with advanced problem-solving strategies in the design and manufacturing space. ChatGPT, for instance, has shown efficacy in mitigating issues such as warping and stringing in the fused filament fabrication (FFF) process, saving both time and material by optimizing computationally multiple parameters efficiently.^{23,24}

In academic contexts, especially in undergraduate studies, it provides a supportive base for information gathering and initial research endeavors.²⁵

In particular, ChatGPT serves as a versatile educational tool in multiple capacities such as tutoring, assisting with research, and supporting teaching activities. Its distinction from other large language models (LLMs) lies in its user-friendly nature, tailored interactions, dialogue-based interface, and affordability. While numerous studies have explored the application of artificial intelligence (AI) in education, including chatbots,²⁶ programming assistance,^{27,28} language models,^{4,29} and NLP tools,³⁰ ChatGPT represents a comparatively recent innovation in the realm of education (Fig. 1).

OpenAI's GPT-4 is an advanced multimodal large language model, constituting the fourth installment in the GPT series. Released on March 14, 2023, it is accessible to the public through the ChatGPT Plus paid chatbot product and OpenAI's API. Leveraging a transformer architecture, ChatGPT-4 employs a two-step approach that involves pre-training on a combination of public data and third-party licensed data to predict subsequent tokens. Subsequently, reinforcement learning is employed, incorporating feedback from both human and AI sources to align with human behavior and adhere to established policies. Experts have noted that the integration of ChatGPT-4 into ChatGPT represents an improvement over its predecessor, ChatGPT-3.5.^{31–35}

Finally, it is worth noting that, in each of these applications, the validity and reliability of ChatGPT's outputs are dependent upon the quality of the training data and system design, and hence, it has been emphasized that it should not serve as a sole resource but be utilized in tandem with other tools and expert insights.

A recurring theme across research findings in different fields is a note of caution regarding the limitations of the model. Despite its utility in offering initial insights, generating reports, and facilitating certain processes, the model's output requires rigorous validation to ensure accuracy and reliability, given its tendency for biases and inaccuracies. Therefore, while ChatGPT shines as a versatile tool with numerous potentials across varied fields, it is imperative that its usage is supplemented and balanced with expert human oversight and additional validating tools to truly harness its capabilities reliably and effectively.

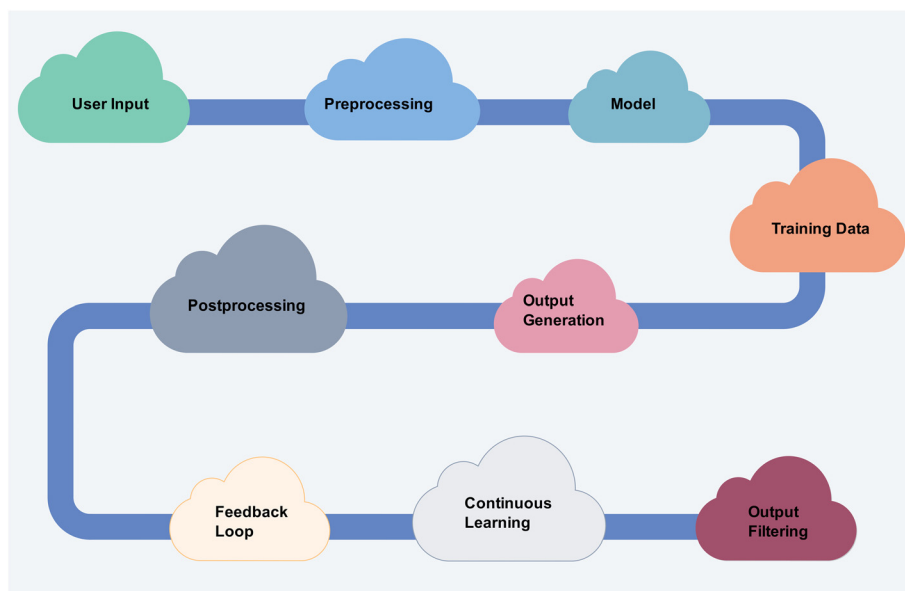


Fig. 1 Illustrative diagram depicting the operational mechanism of ChatGPT.

Progressive impact of AI and LLMs: from data handling to creative insight

In the era permeated by the digital revolution and artificial intelligence (AI), large language models (LLMs), like ChatGPT-4, have emerged as pivotal allies, providing transformative impacts across various domains, thereby enhancing and augmenting human capabilities in unprecedented ways. The convergence of linguistic understanding, facilitated by LLMs, and the adaptive learning and problem-solving capacities of AI have significantly accelerated our ability to interpret, innovate, and address multifaceted challenges in science.

Level 1: data management and basic processing

Embarking upon the elementary capabilities, AI and LLMs proficiently cater to the vital requirements of data management and basic processing, executing core functions such as data storage, retrieval, and preliminary processing operations, thereby establishing a structured data ecosystem.^{36–38}

Level 2: analytical insight and decision support

Advancing towards analytical insight and decision support, AI and LLMs unveil their capacity to detect patterns and irregularities within data, concurrently enabling the synthesis of insightful recommendations to fortify decision-making processes.^{39–41}

Level 3: interaction and automation

In the realm of interaction and automation, AI and LLMs shine brightly, allowing them to both understand and create human language. This is not just about chatting with them, but also about simplifying and speeding up a wide range of

regular, rule-following tasks through automation. Essentially, it is all about making conversations smoother and work processes more streamlined, creating an effortless communication between humans and technology, and making operations run more smoothly.^{42,43}

Level 4: problem-solving and continuous learning

Transcending to problem-solving and continuous learning, AI and LLMs demonstrate a remarkable ability to tackle intricate challenges by analyzing multiple elements. Furthermore, these systems are designed to constantly improve their methods, optimizing their performance. This ongoing refinement process endows them with increasingly accurate prediction capabilities and heightened problem-solving skills.⁴⁴ Continual learning, also known as lifelong learning,^{45,46} in the context of machine learning, refers to the ability of a system to continually learn and adapt to new information over time without forgetting previously acquired knowledge. This concept is particularly important as it aims to mimic the human ability to learn continuously throughout life.

Key characteristics of continual learning

Incremental learning. The ability to learn from new data that may not have been available during the initial training phase.

Avoidance of catastrophic forgetting. Traditional machine learning models, when trained on new data, tend to forget the knowledge gained from previous data, a phenomenon known as catastrophic forgetting. Continual learning aims to overcome this by retaining the knowledge gained from previous learning phases.

Adaptability to new tasks. The system should be able to adapt to new tasks or changes in the data distribution without the need for extensive retraining from scratch.

Level 5: creativity and aspiring general intelligence

Previously dominated solely by human intellect, this level of intelligence now witnesses the emergence of advanced AI and LLMs as co-inhabitants. At this level, AI and LLMs explore the artistic domains of creativity, generating innovative content and tentatively navigating through avenues that lead toward mastering generalized problem-solving across various fields. This implies a prospective future where machines not only emulate but perhaps mirror multifaceted, human-like intellectual capabilities, thereby melding machine and human intelligence in unison.^{47,48}

Oxygen evolution reactions

Hydrogen production plays a crucial role in clean, low-carbon economies, thanks to its high energy density and effectiveness as an energy carrier. Some countries have outlined strategies for hydrogen and fuel cell vehicles, highlighting the global interest in efficient hydrogen production. Traditionally, hydrogen has been produced through coal gasification, a method that causes carbon monoxide contamination and still depends on fossil fuels. A promising alternative is electrocatalytic water splitting.⁴⁹ This method is clean and sustainable, converting renewable energy into green chemical fuels. The process involves splitting water into hydrogen and oxygen through two half-cell reactions: the hydrogen evolution reaction (HER) at the cathode and the oxygen evolution reaction (OER) at the anode.⁴⁹ The HER is a two-electron transfer process, while the OER, a four-electron transfer process, is kinetically less favorable. The OER holds substantial importance in the realm of sustainable energy production, particularly due to its role in providing low-cost electrons essential for the HER.⁴⁹ This aspect of the OER is critical because it facilitates a more economic and efficient process for hydrogen generation. By producing electrons at a lower cost, the OER enables the HER to occur under conditions that are financially feasible and sustainable.⁴⁹ This relation between the OER and the HER is a cornerstone in advancing hydrogen production technologies, making them more accessible and viable for broader applications in clean energy systems. The ability of the OER to supply inexpensive electrons thus plays a pivotal role in enhancing the overall efficiency and cost-effectiveness of hydrogen production, a key factor in the transition towards greener and more sustainable energy sources. Consequently, there has been significant research into efficient electrocatalysts for the OER. Traditional OER catalysts have relied on iridium oxide (IrO₂) or ruthenium oxide (RuO₂).⁴⁹ However, their high cost and limited availability pose economic challenges to widespread industrial use. To address this, there has been a growing interest in exploring low-cost transition metal-based catalysts, especially in alkaline media, due to their promising intrinsic activity and stability for the OER. These advancements are part of a broader effort to make hydrogen production more sustainable and economically viable.

We currently assume that we are at level 4. In the following subsection, we aim to assess the significance of AI and LLMs in aiding scientific endeavors, particularly in the field of accelerating OERs.

Materials and methods

Utilization of OpenAI's ChatGPT

In this investigation, we employed OpenAI's ChatGPT 4.0, an AI-driven language model, to assist in various aspects of the research process including literature review, hypothesis formulation, and data interpretation. ChatGPT 4.0's advanced natural language processing capabilities were instrumental in providing comprehensive, up-to-date information and facilitating the understanding of complex scientific concepts.

Interaction with ChatGPT

Interactions with ChatGPT were facilitated through the OpenAI platform's web-based interface. The language model was engaged with a series of structured prompts crafted to obtain specific information pertinent to the research topics at hand. Each query was meticulously designed to extract detailed explanations, generate textual data, and interpret research findings.

Parameters and customization

The default settings of ChatGPT were utilized without modification for all interactions. This approach ensured consistency across the information retrieval sessions. The model's parameters including response length were automatically managed by the AI to provide optimal output based on the complexity and requirements of each prompt.

Documentation of ChatGPT sessions

Every session with ChatGPT was systematically documented, capturing both the input prompts and the AI-generated responses. This record-keeping was conducted to maintain a comprehensive trail of the AI's contribution to the research process, thereby allowing for reproducibility and transparency.

Ethical considerations and data privacy

The use of ChatGPT 4.0 adhered to ethical guidelines, with no requirement for ethical approval since the AI does not involve human participants or personal data. All generated data from ChatGPT was non-sensitive and strictly related to publicly available scientific information.

Results and discussion

Empowering sustainable energy research: ChatGPT-4 as a revolutionary assistant for developing efficient OER catalysts

Hydrogen production is pivotal for clean energy, traditionally relying on coal gasification but now shifting towards sustainable electrocatalytic water splitting. This method splits water

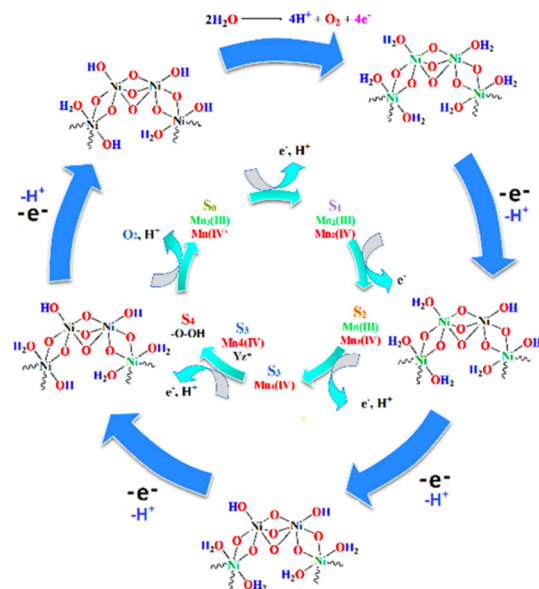
into hydrogen and oxygen, with the oxygen evolution reaction (OER) being crucial for efficient hydrogen generation.⁴⁹ The HER involves a two-electron transfer, whereas the OER, a four-electron transfer, is kinetically slower but crucial in sustainable energy for supplying low-cost electrons vital for the HER.⁴⁹ Recent research focuses on affordable, efficient electrocatalysts for the OER, moving away from costly materials to enhance hydrogen production's sustainability and economic feasibility. ChatGPT-4 is a revolutionary assistant for developing efficient OER catalysts. In the natural realm, organisms such as cyanobacteria, algae, and plants employ a comparable oxygen-evolving complex (OEC) found within photosystem II, a membrane-protein complex responsible for the light-driven oxidation of water during oxygenic photosynthesis.^{50–53} The biological OEC consists of a Mn–Ca cluster that exhibits exceptional characteristics in water oxidation.^{54–57} It displays an exceedingly low overpotential of only 20 mV and operates at a high turnover frequency, releasing between 25 and 90 molecules of O₂ per second.^{54,55} The mechanism proposed by Kok, extensively accepted in the scientific community, outlines the progression of OEC through five distinct states: S₀ to S₄. S₄ represents the most oxidized state, while S₀ denotes the most reduced state. The absorption of photons by photosystem II triggers the transition of the system from state S₀ to S₄. However, due to its instability, S₄ reacts with water, resulting in the formation of O₂, as indicated in ref. 56 and 57. A recent study has focused⁵⁸ on the electrocatalytic activity of nickel (hydr)oxide in the OER at an extremely low overpotential.⁵⁸ The results indicated that the catalyst displayed remarkable OER activity with an impressively low overpotential of merely 90–120 mV.⁵⁸ Additionally, the Tafel slope was measured to be 297 mV per decade. These findings highlight the potential of nickel (hydr)oxide as a promising candidate for the development of efficient OER catalysts in sustainable energy systems (Scheme 1).⁵⁸

To gain insights into the observed OER activity, we employed *in situ* Raman spectroscopy, which provided valuable information about the underlying mechanism. The results indicated that the OER activity at such low overpotentials is related to charge accumulation, drawing parallels to the biological OEC. The proposed association between the OER activity and the charge accumulation opens up exciting possibilities for exploring novel electrocatalysts that contribute to sustainable energy generation.⁵⁸ Thus, the study illuminates the cost-effective and efficient nature of nickel (hydr)oxide as a catalyst for OERs.⁵⁸

The catalyst demonstrated remarkable OER activity at a minimal overpotential, and the proposed link between the OER activity and the charge accumulation establishes a solid foundation for future research in the field of sustainable energy storage.⁵⁸ Thus, even though the initial idea did not originate from a machine, we evaluated GPT 4.0 to further enhance and refine the concept:

We asked ChatGPT 4.0:

- Read it⁵⁸ and write ideas to improve the idea from the increase in activity to study the details.



Scheme 1 During the OER, the Kok cycle operates alongside a biological site, while a separate OER cycle occurs for a Ni₄O₄ complex. Initially, water molecules bind to the Ni(II) active sites. These Ni(II) sites are then oxidized to Ni(III), which are pivotal in facilitating the OER, ultimately yielding O₂, H⁺, and electrons. Concurrently, Ni(III) is reduced back to Ni(II), resetting the catalyst for a subsequent identical cycle. The liberated H⁺ may participate in other chemical processes such as the hydrogen evolution reaction (HER). The electrons produced in this cycle become available for various reduction reactions. Reproduced with permission from ref. 58 Copyright (2023) American Chemical Society.

ChatGPT 4.0 wrote (*in italics*):

The research has been well codified and the ideas presented systematically. However, for further improvement in the study, several aspects can be considered:

1. Material synthesis variations: *The study can explore synthesizing nickel oxyhydroxide under different conditions (e.g., temperature, pressure, pH) or using different methods to investigate how these variables impact the OER activity. This could help in optimizing the synthesis process for superior results.*

2. Material modifications: *The inclusion of other metal ions or doping agents in the nickel (hydr)oxide catalyst could be considered. This could potentially enhance the catalytic activity and efficiency of the OER.*

3. Multi-technique characterization: *Apart from Raman spectroscopy, it could be beneficial to employ other characterization techniques such as X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), or transmission electron microscopy (TEM) for a more comprehensive understanding of the material's structural and morphological properties.*

4. Kinetic studies: *Detailed kinetic studies into the rate of the OER could provide further insight into the efficiency of the catalyst. Understanding the reaction kinetics could give clues to improving the catalyst design and operation.*

5. Comparison with other catalysts: *Comparing the performance of nickel oxyhydroxide with other well-known OER catalysts under similar conditions could provide a better understanding of its efficiency and competitive advantage.*

6. Real-world testing: Finally, testing the catalyst in real-world conditions or a scaled-up setup could provide practical insights into its performance and durability. It could also lead to a better understanding of the challenges that might be encountered when scaling up the technology.

7. Theoretical modelling: Complementing the experimental work with theoretical modeling could provide a deeper understanding of the reaction mechanism and the role of Ni(II) to Ni(III) transition in OER. Density functional theory (DFT) calculations or similar computational chemistry methods could be employed to support experimental findings.

8. Exploring Ni(IV) role: As mentioned in the study, some researchers believe that the active state for OER may be Ni(IV). Hence, further exploration of the role of Ni(IV) in OER could be beneficial and could potentially lead to even more efficient catalysts.

9. Stability studies: Long-term stability studies can provide insights into the durability of the catalyst. Understanding how the catalyst's performance changes over time under continuous operation can help in assessing its feasibility for practical applications.

10. Investigating the role of the support material: The stability of Ni(III) sites was found to depend on the support material. Further investigations could be conducted to understand this relationship and how different support materials might affect catalyst performance.

11. Environmental impact assessment: A study could be conducted to understand the environmental impact of the synthesis, usage, and disposal of the catalyst.

12. Electrode material studies: Different electrode materials could be tested to see if they impact the performance of the catalyst.

13. Particle size effects: The catalyst's particle size could affect its performance. Studies could be conducted to determine the impact of particle size on OER activity.

14. Use of nanostructured catalysts: Nanostructuring the catalyst could increase its active surface area, which could potentially enhance its performance.

15. Catalyst structure–activity relationship: A detailed investigation into the relationship between the catalyst's structure and its performance could provide valuable insights for the design of more efficient catalysts.

16. Investigation of the charge transfer process: The charge transfer process could be studied in more detail to understand its role in the OER.

17. Electrocatalyst poisoning studies: Studies could be performed to determine how resistant the catalyst is to poisoning by impurities.

18. Electrochemical impedance spectroscopy (EIS) studies: EIS could be used to study the kinetics of the electrochemical reaction and the interaction between the electrode and electrolyte.

19. Study of mass transport effects: The role of mass transport in the overall reaction rate could be investigated.

20. Investigation of multi-electron transfer reactions: A detailed study could be conducted on the catalyst's ability to facilitate multi-electron transfer reactions, which are typically challenging.

21. Co-catalyst impact study: Implementing a co-catalyst and studying its impact on the efficiency of the OER reaction could be beneficial.

22. Investigation of the effect of catalyst loading: The amount of catalyst loaded on the electrode could influence the reaction kinetics. This aspect could be studied in detail.

23. Study of the effect of gas bubble evolution: The gas evolution during OER could affect the reaction, and this aspect could be investigated.

24. Investigating the use of additives: Additives could be utilized in the electrolyte solution to enhance the reaction rate or stability of the catalyst.

25. Investigation of the effect of electrolyte concentration: Studies could be performed to understand how the concentration of the electrolyte affects the OER.

26. Study of the effect of stirring: The stirring rate can influence mass transport during the OER. This aspect could be studied in detail.

27. Investigation of the catalyst's stability in different atmospheres: The catalyst's stability could be tested in different atmospheres (e.g., air, pure oxygen, nitrogen) to understand its suitability in different working conditions.

28. Use of other advanced characterization techniques: Techniques like high-resolution transmission electron microscopy (HR-TEM), scanning transmission electron microscopy (STEM), energy-dispersive X-ray spectroscopy (EDX), and electron energy loss spectroscopy (EELS) could be used to gain further insights into the catalyst's structure and composition.

29. Simulation studies: Simulation studies could be done to predict the catalyst's behavior under different working conditions.

30. Cost analysis: A detailed cost analysis could be conducted to determine the feasibility of the catalyst for large-scale applications.

ChatGPT 4.0 could organize the ideas (Fig. 2):

1. Material synthesis and modification:

- Material synthesis variations (1)
- Material modifications (2)
- Investigating the role of the support material (10)

2. Characterization techniques:

- Multi-technique characterization (3)
- Use of other advanced characterization techniques (28)

3. Kinetic and mechanistic studies:

- Kinetic studies (4)
- Theoretical modelling (7)
- Exploring Ni(IV) role (8)
- Investigation of multi-electron transfer reactions (20)
- Study of mass transport effects (19)
- Electrochemical impedance spectroscopy (EIS) studies (18)
- Investigation of the charge transfer process (16)

4. Comparative and performance evaluation:

- Comparison with other catalysts (5)
- Real-world testing (6)
- Stability studies (9)
- Environmental impact assessment (11)

5. Catalyst optimization and modification:

- Electrode material studies (12)
- Particle size effects (13)

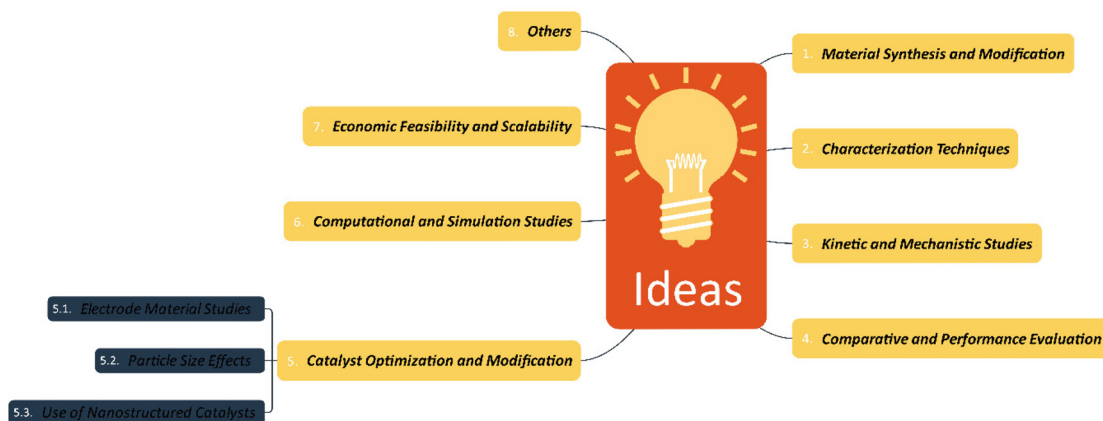


Fig. 2 ChatGPT 4.0 could organize those 39 ideas for further improvement in the study (see ref. 58). Details of catalyst optimization and modification are shown.

- Use of nanostructured catalysts (14)
- Catalyst structure–activity relationship (15)
- Electrocatalyst poisoning studies (17)
- Co-catalyst impact study (21)
- Investigation of the effect of catalyst loading (22)
- Investigating the use of additives (24)
- Investigation of the effect of electrolyte concentration (25)
- Study of the effect of stirring (26)
- Investigation of the catalyst's stability in different atmospheres (27)

6. Computational and simulation studies (Fig. 3):

- Simulation studies (29)

7. Economic feasibility and scalability:

- Cost analysis (30)

8. Others:

- Study of the effect of gas bubble evolution (23)

ChatGPT 4.0 has the potential to offer additional ideas, but it should be noted that some of them might be repetitive. While experts can propose all of these 30 ideas, this compilation is valuable and can provide valuable assistance to researchers. All these ideas (proposals) or at least many of them could be promising and helpful in improving the activity or understanding of the system. Asking ChatGPT 4.0 to write novel ideas results in:

1. **Quantum dot sensitization:** Experiment with sensitizing nickel oxyhydroxide surfaces with quantum dots, like CdSe or

PbS, to enhance light absorption and promote photo-induced charge separation. This could improve the efficiency of OER in photoelectrochemical cells.

2. **Piezoelectric material integration:** Integrate piezoelectric materials with nickel oxyhydroxide catalysts to harness mechanical vibrations (from wind or acoustic waves) for enhancing charge density and OER activity.

3. **Thermoelectrically enhanced OER:** Investigate the use of thermoelectric materials in conjunction with nickel oxyhydroxide to utilize heat gradients (possibly from industrial waste heat) to drive or enhance the OER process.

4. **Smart responsive catalyst coatings:** Develop smart coatings for nickel oxyhydroxide catalysts that can change their properties in response to external stimuli (like pH, temperature, or light), allowing dynamic control over the OER process efficiency.

5. **Acoustic field application:** Apply targeted acoustic fields to the electrolysis setup to stimulate the catalyst surface. This novel approach could influence molecular arrangements or enhance reaction kinetics on the nickel oxyhydroxide surface.

6. **Electrodynamics field manipulation:** Implement a system where dynamic electrodynamics fields (alternating electromagnetic fields) are used to constantly modify the orientation of nickel oxyhydroxide molecules, potentially altering their catalytic properties and enhancing OER efficiency.

7. **Quantum tunneling enhancement:** Explore ways to exploit quantum tunneling effects at the nano-scale to enhance electron

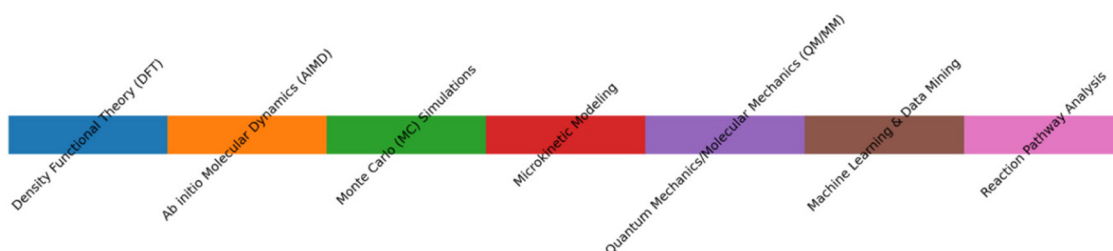


Fig. 3 Details of computational and simulation studies for further improvement in the study (see ref. 58).

transfer rates in the nickel oxyhydroxide catalyst. This could involve engineering the catalyst at a quantum level to optimize its electronic properties for OER.

8. Catalyst self-assembly under microgravity: Conduct experiments to study the self-assembly of nickel oxyhydroxide catalysts in a microgravity environment. This could lead to the discovery of novel catalyst structures that are not possible to achieve under Earth's gravity.

9. Bio-hybrid systems: Investigate the integration of biological components, such as specific enzymes or microorganisms, with nickel oxyhydroxide. These bio-hybrid systems could utilize biological mechanisms to enhance the catalytic efficiency or stability of the material.

10. 4D printing of catalyst structures: Use 4D printing technology to create nickel oxyhydroxide structures that can change shape or properties in response to environmental stimuli (like temperature, light, or pH), potentially offering a dynamic control mechanism for OER efficiency.

11. Catalyst 'healing' using smart nanobots: Develop microscopic nanobots capable of 'healing' or reconstructing the nickel oxyhydroxide catalyst structure in situ. These nanobots could actively repair defects or degradation in the catalyst, prolonging its life and efficiency.

12. Cryogenic treatment of catalysts: Experiment with cryogenic treatment of the nickel oxyhydroxide catalysts before their use in OER. This unconventional approach might induce changes in the crystalline structure or surface properties, influencing catalytic activity.

13. Exploring non-Newtonian fluid dynamics in electrolytes: Use non-Newtonian fluids as electrolytes in the OER process and study their interaction with nickel oxyhydroxide. The unique flow characteristics of these fluids might offer new ways to enhance mass transfer and catalytic efficiency.

In addition, ChatGPT 4.0 could focus on each case and explain it in detail. For example, we asked it:

explain: "18. Exploring Ni(IV) Role"

ChatGPT 4.0 wrote (*in italics*):

In the context of the research presented, "exploring Ni(IV) role" refers to the examination or investigation of the role of the nickel ion in the IV oxidation state, specifically in the OER process. The primary focus of this research is the OER catalytic activity of nickel oxyhydroxide, especially during the transition from the Ni(II) to Ni(III) oxidation state. However, it is mentioned that some recent research suggests that the active state for OER may indeed be Ni(IV). Hence, exploring the role of Ni(IV) could potentially lead to even more efficient catalysts.

Ni(IV) is an oxidation state of nickel. While Ni(II) and Ni(III) are more common and have been extensively studied, Ni(IV) is less common and less understood. It is believed that Ni(IV) may offer higher catalytic activity for OER, but this requires further investigation.

Exploring the role of Ni(IV) in OER would involve conducting experiments to determine whether Ni(IV) is indeed the active state for OER and understanding how it interacts with other components of the system during the reaction. This could involve a variety of experiments, including but not limited to, electro-

chemical tests, spectroscopy, and microscopy, to understand the detailed mechanisms at play.

Further investigations could reveal more about the potential advantages of Ni(IV) in OER, such as improved efficiency, lower overpotential requirements, or enhanced stability. This could lead to the development of more effective catalysts for OER, which would be beneficial for a variety of applications in energy storage and conversion technologies, such as water splitting for hydrogen generation, and rechargeable metal-air batteries.

In the next step, based on one of the ideas by the ChatGPT, we investigated a simple model for the system:

On a bullet page, there are bullets with positive charges as Ni(III) ions, uniformly spaced and at a fixed distance from each other. Which bullets should we neutralize toward Ni(II) first to reduce the system's energy due to Coulomb repulsion with minimal speed? The coordinates of the bullets are given as (i, j) , where i and j are integers ranging from 0 to 100. The speed of neutralization related to the OER is inversely proportional to the number of neighboring bullets. This means that bullets with more neighbors will be neutralized faster. It has a direct relationship with the total charge of the system. As the positive charge decreases over time, the reaction speed also decreases linearly. The curve of coulombic energy reduction over time was plotted. Coulomb's law, states that the force of attraction or repulsion between two charged bodies (Ni(III)–Ni(III) interaction) is directly proportional to the product of their charges and inversely proportional to the square of the distance between them. The coulombic energy of a system of charges is the sum of the potential energies of all pairs of charges. The potential energy of a pair of charges (U) is given as follows (eqn (1)):

$$U = k_e \frac{q_1 q_2}{r} \quad (1)$$

where k_e is the Coulomb constant, q_1 and q_2 are the charges, and r is the distance between them.

In this problem, there is a grid of bullets with positive charges, uniformly spaced and at a fixed distance from each other. The coordinates of the bullets are given as (i, j) , where i and j are integers ranging from 0 to 100. We can assume that the distance between two adjacent bullets is 1 unit, and that the charge of each bullet is 1 unit. Therefore, the Coulombic energy of the system is (eqn (2)):

$$E = \frac{k_e}{2} \sum_{i=0}^{100} \sum_{j=0}^{100} \sum_{k=0}^{100} \sum_{l=0}^{100} \frac{1}{\sqrt{(i-k)^2 + (j-l)^2}} \quad (2)$$

where we divide by 2 to avoid double counting the pairs.

The question is which bullets should we neutralize first to reduce the system's energy due to Coulomb's repulsion with minimal speed. The speed of neutralization is inversely proportional to the number of neighboring bullets. This means that bullets with more neighbors will be neutralized faster. It has a direct relationship with the total charge of the system. As the positive charge decreases over time, the reaction speed also decreases linearly.

One possible strategy to minimize the speed of neutralization is to neutralize the bullets that have the highest potential energy first. This way, we can reduce the total charge and energy of the system faster, and slow down the reaction accordingly. To find the bullets with the highest potential energy, we can calculate the potential energy of each bullet as follows (eqn (3)):

$$U_i = k_e \sum_{k=0}^{100} \sum_{l=0}^{100} \frac{1}{\sqrt{(i-k)^2 + (j-l)^2}} \quad (3)$$

where (i, j) are the coordinates of the bullet. Then, we can sort the bullets in descending order of their potential energy and neutralize them one by one according to this order.

To plot the curve of coulombic energy reduction over time, we need to keep track of how much energy and charge are left in the system after each neutralization step. We also need to know how much time it takes to neutralize each bullet, which depends on the number of neighbors and the total charge. Using these formulas, ChatGPT (browse with Bing) can write a Python program to simulate the neutralization process and plot the curve of coulombic energy reduction over time (see ESI† for a Python code). Although the model is very simple, a comparison of this data and experimental data shows verisimilar trends between the model and experimental data (Fig. 4).

As expertise in highly specialized fields such as computational chemistry is not always readily accessible, ChatGPT can serve as an invaluable resource. For instance, it can illuminate for an experimentalist how density functional theory (DFT) holds great promise for their work. It can elucidate that DFT offers profound insights into the electronic configurations and potential energy landscapes of complex materials such as nickel-based catalysts used in OERs.

Furthermore, ChatGPT can highlight how DFT can predict the most stable structures of nickel hydroxides and their corresponding oxidized phases, which are often subjects of debate in the scientific community. By simulating the elec-

tronic structure, ChatGPT can guide experimentalists toward understanding the nuanced properties that dictate catalytic activity. Moreover, ChatGPT can detail how DFT can assist in visualizing the reaction pathways and the energetic feasibility of various steps in the OER process. This can be especially enlightening for those who are more familiar with hands-on laboratory work rather than theoretical calculations. Additionally, for experimentalists interested in the effects of dopants such as Fe, ChatGPT can describe how DFT is capable of teasing out the interactions at the atomic level, which enhance or impede the catalytic process. It can explain that through DFT, one can discern the electronic changes induced by doping and how these changes translate into real-world catalytic performance. In the realm of energy storage and conversion, where efficiency is paramount, ChatGPT can also stress the importance of DFT in predicting and optimizing the energetics of the catalytic system. This includes understanding overpotentials, Tafel slopes, and the kinetics of electron transfer—all of which are critical parameters for a catalyst's efficiency. By providing a bridge between the experimental and theoretical worlds, ChatGPT can help experimentalists leverage DFT to enhance their understanding and development of better catalysts. This collaboration between computational predictions and empirical data can lead to the accelerated discovery of more effective and sustainable energy solutions.

The application of density functional theory (DFT) to the nickel system discussed earlier

To specifically address the application of density functional theory (DFT) to the nickel system discussed earlier, here's how DFT could be particularly useful (Fig. 5):

1. **Understanding electronic structure:** DFT can accurately determine the electronic structure of both β -NiO(OH) and γ -NiO(OH). This is essential because the OER activity hinges on the electronic states of Ni(II) and Ni(III). DFT can help in determining the density of states, band structure, and the precise energy levels involved in the redox reactions.

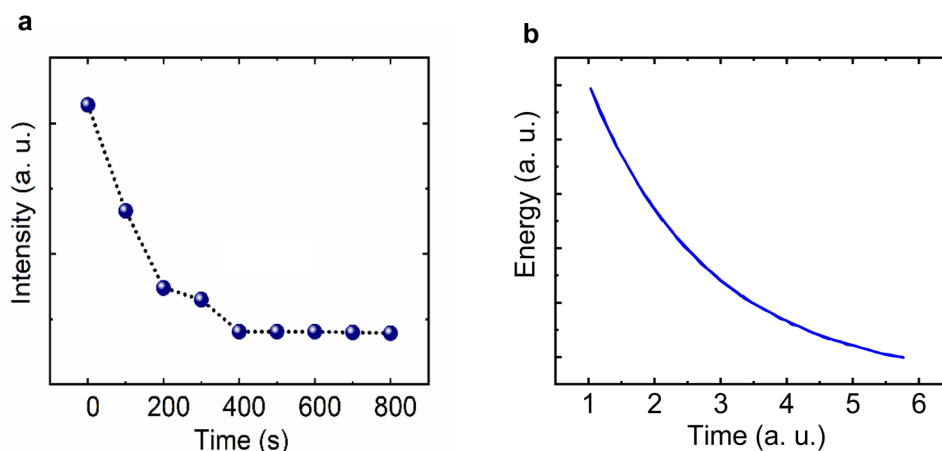


Fig. 4 Observed changes in the intensity of peaks at 470 nm recorded by Raman spectroscopy⁵⁸ for NiO(OH) (a). Changes in energy vs. time for the modeled system proposed by ChatGPT (b).

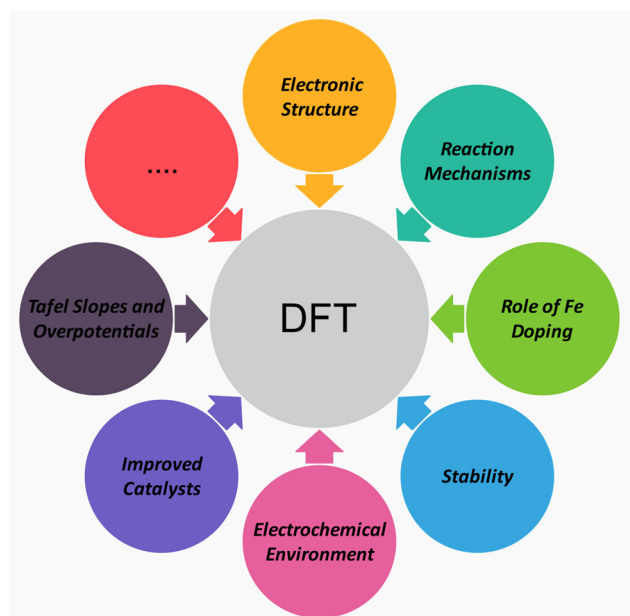


Fig. 5 Schematic diagram showing how DFT can be useful for further improvement in the study (see ref. 58).

2. Elucidating reaction mechanisms: By mapping out the potential energy surface for the OER on $\text{NiO}(\text{OH})$, DFT can help identify transition states and intermediate species that are difficult to detect experimentally. This information is crucial for understanding the step-by-step mechanism of the OER process.

3. Assessing the role of Fe doping: For the Fe-doped $\text{Ni}(\text{OH})_2$ systems, DFT can predict how Fe incorporation affects the electronic properties and catalytic activity. It can provide insights into the electronic interactions between Fe and Ni ions and the resulting impact on the OER performance.

4. Predicting structural stability: DFT can predict which of the proposed structures for $\beta\text{-NiO}(\text{OH})$ and $\gamma\text{-NiO}(\text{OH})$ are more thermodynamically stable under OER conditions. This is vital for understanding the durability and lifetime of the catalyst.

5. Evaluating the effect of the electrochemical environment: DFT can simulate the influence of the KOH electrolyte on the stability and reactivity of $\text{NiO}(\text{OH})$. Solvent effects and ion interactions can be incorporated to some extent, providing a more realistic depiction of the catalyst in operation.

6. Investigating the Jahn–Teller distortion: The Jahn–Teller effect is associated with the degeneracy lifting in certain electronic states of ions. DFT can provide detailed information on the structural changes associated with the Jahn–Teller distortion in $\text{Ni}(\text{III})$ sites during the OER.

7. Designing improved catalysts: Based on the insights from DFT calculations, modifications to the catalyst structure or composition can be proposed to enhance OER activity, stability, and selectivity. DFT can guide the synthesis of novel materials with improved properties.

8. Calculating Tafel slopes and overpotentials: DFT can compute activation energies for the OER steps, which are directly related to the Tafel slopes and overpotentials. These calculations

can help explain the observed experimental values and suggest ways to minimize energy losses.

In summary, DFT is a powerful tool for providing atomistic and electronic insights into the behavior of Ni-based catalysts in OER. It can help resolve controversies regarding the structure of oxidized phases, clarify reaction mechanisms, and guide the design of more efficient catalysts.

Explain point 3 more:

Certainly. The role of Fe doping in the context of nickel hydroxide-based catalysts for the oxygen evolution reaction (OER) is an important area of study, as Fe (iron) can significantly impact the electrochemical properties of the material.

1. Catalytic activity enhancement: Fe ions, when incorporated into the nickel hydroxide lattice, can act as active sites themselves or modulate the existing nickel active sites. This can lead to an enhancement in the catalytic activity due to a change in the electronic structure, providing more favorable pathways for the OER to proceed. Fe doping may alter the oxidation state distribution and the electronic conductivity of the material, both of which are crucial for improving the efficiency of the OER.

2. Stabilization of $\text{Ni}(\text{III})$ species: Research indicates that Fe doping may help stabilize higher oxidation state species of nickel, such as $\text{Ni}(\text{III})$ or even $\text{Ni}(\text{IV})$, which are believed to be active for the OER. The presence of Fe could create a local environment that stabilizes these oxidation states, preventing them from disproportionating or reducing back to lower oxidation states.

3. Structural modification: Introducing Fe into the $\text{Ni}(\text{OH})_2$ structure can lead to changes in the lattice parameters and the introduction of strain or defects. These structural modifications can affect the adsorption of intermediates and the desorption of O_2 , two critical steps in the OER mechanism.

4. Electrical conductivity: Fe doping can improve the electrical conductivity of Ni-based catalysts by creating a more conductive pathway through the material. This enhancement in conductivity ensures that electrons can move more freely through the catalyst, which is essential for efficient electrocatalytic processes.

5. Overpotential reduction: The inclusion of Fe may reduce the overpotential required for the OER. Overpotential is the extra voltage beyond the thermodynamic requirement needed to drive the reaction at a noticeable rate. A lower overpotential means the reaction can proceed at a lower applied voltage, increasing the energy efficiency of the process.

6. Durability and cycling stability: Catalysts that undergo the OER often suffer from degradation over time, which manifests as a loss of activity and changes in the structure. Fe doping has been shown to improve the durability and cycling stability of nickel-based catalysts, likely due to the more robust structure that results from Fe incorporation.

By studying Fe doping in nickel hydroxide systems, researchers can uncover the fundamental reasons behind these observed improvements in OER performance. It is this improved understanding that will guide the design of next-generation electrocatalysts that are not only more efficient but also more durable and sustainable for long-term energy applications.

Furthermore, ChatGPT can be an asset to those with theoretical expertise by demonstrating how experimental work can validate DFT predictions. It can guide a theoretical scientist in understanding how empirical data from experiments can corroborate the theoretical models and computational results, thereby reinforcing the reliability of their DFT analyses.

It is crucial to highlight that ChatGPT 4.0 can assist in drafting a proposal, elaborating on the topic, analyzing data, planning timelines and budgets, composing theses and papers, and choosing an appropriate journal for the manuscript (see ESI†). Additionally, ChatGPT 4.0 was utilized for the analysis of three other catalysts, details of which can be found in the ESI.†^{59–61}

We posit that AI holds the potential to drive substantial advancements in the field of catalysis in the future. Predictive modeling through AI accelerates the discovery and refinement of catalysts by foretelling their behavior under diverse conditions, making it a vital tool in modern catalysis. This dovetails with automated experimentation where AI-driven robotic systems facilitate high-throughput testing of a broad spectrum of catalysts under different conditions, expediting both discovery and optimization. The colossal data generated in these processes can be meticulously analyzed by AI to unveil new insights, discern patterns, and enhance catalytic processes. Furthermore, AI is instrumental in simulating molecular interactions at the atomic level, a cornerstone for understanding and improving catalyst functionality. Real-time monitoring and control by AI algorithms ensure optimal performance by adjusting the conditions instantaneously. This seamless monitoring extends into the domain of materials discovery, where AI accelerates the process by predicting the properties of potential catalytic materials, conserving both time and resources. The ripple effect of AI's involvement also touches the educational sphere, aiding in the development of tools and training programs to foster a deeper understanding of catalysis. Knowledge sharing is another facet amplified by AI, fostering a community of researchers and practitioners propelling towards collective advancements in the field. Environmental monitoring becomes more streamlined with AI, promoting sustainable practices by assessing the environmental impacts of catalytic processes. Cost reduction is a significant boon, with AI optimizing processes and curtailing R&D time, thereby reducing costs associated with catalytic processes. The journey of discovery continues with AI analyzing vast chemical libraries and datasets to predict new catalysts with desired properties, an invaluable asset for advancing catalysis. The optimization of catalytic processes is achieved by fine-tuning reaction conditions such as temperature, pressure, and pH through AI algorithms. Understanding complex catalytic reaction mechanisms is simplified with AI, providing models for reaction pathways and intermediate species based on data analysis. In industrial settings, predictive maintenance enabled by AI reduces downtime and enhances efficiency by scheduling timely maintenance or replacement of catalysts. Tailoring catalysts for specific reactions, a crucial requirement in industries

such as pharmaceuticals and fine chemicals, is facilitated by AI. The umbrella of sustainable and eco-friendly catalysis is expanded with AI aiding in developing catalysts operating under milder conditions, reducing both energy consumption and environmental impact. The integration of AI with high-throughput experimentation accelerates innovation cycles through a closed-loop system of hypothesis, testing, and refinement, embodying a new era of data-driven insights. Collaborative research is bolstered as AI aggregates and analyzes data from different laboratories, facilitating a more coordinated and comprehensive research effort. Lastly, economic analysis and forecasting through AI help industries make informed decisions regarding the adoption of new catalysts or technologies, underlining the pervasive impact of AI across the entire spectrum of catalysis.

Among these cases, real-time analysis and adaptation allows AI-driven robotic systems to offer real-time analysis during experiments, dynamically adapting conditions for optimized results, and facilitating an efficient exploration of catalytic behaviors. Expansive exploration through automation allows for tireless traversing of a vast catalytic landscape, unveiling potential catalysts faster and more accurately. Precision and reproducibility, hallmark traits of robotic systems, generate high-fidelity data crucial for reliable conclusions, thus accelerating the validation of new catalysts. Indeed, human error and directional errors can be eliminated or significantly reduced through the use of robots and artificial intelligence technologies. In addition, robots, programmed to follow precise instructions, can execute tasks with a level of accuracy and consistency that humans might find challenging to maintain over extended periods. Additionally, AI technologies can analyze vast amounts of data to make accurate decisions and provide guidance, reducing the likelihood of errors in judgment or direction that might occur due to human oversight or biases. Through a combination of robotic automation and intelligent data analysis, many processes can be optimized to minimize the occurrence of errors and improve the overall efficiency and effectiveness. Algorithmic experiment design, steered by sophisticated algorithms, rationalizes the allocation of resources based on research priorities, accelerating the trajectory toward impactful discoveries. Continuous learning and evolution are exemplified as AI algorithms evolve with accumulating data, refining predictive models, and fostering a progressively insightful exploration of catalysis. Collaborative robotics enables multiple robotic systems to operate in tandem, sharing data and insights, creating a collective intelligence that significantly accelerates discovery and optimization in catalysis. Virtual reality (VR) interface integration provides researchers an intuitive oversight over automated experimentation, embodying a harmonious human-machine collaboration that leverages the imaginative capacity of humans with the computational prowess of AI. Global research networks, facilitated by automated experimentation, enable data sharing across geographical boundaries, propelling a holistic and inclusive advancement in catalysis research, transcending institutional silos.

Generative pre-trained transformers (GPT) like GPT-4 represent the forefront of advancements in natural language processing, offering unprecedented capabilities in generating human-like text. These models have revolutionized various fields, from customer service automation to creative writing assistance. However, despite their impressive abilities, it is crucial to acknowledge and understand their inherent limitations. These limitations not only shape the way these models should be utilized but also highlight areas for future improvement and ethical considerations. The following points delve into these key limitations in more detail.

Lack of true understanding and contextual comprehension: A primary limitation of GPT-4 and similar models is their lack of real understanding. They generate responses based on pattern recognition from their training data, not actual comprehension. This means that while they can produce text that appears coherent, they might not truly grasp the meaning or context, especially in complex or nuanced discussions. As a result, this can lead to responses that are factually inaccurate, irrelevant, or even nonsensical.⁶²

Biases and offensiveness in outputs: Another significant concern is the tendency of these models to reflect biases and offensive content found in their training data. Since they learn from a vast array of internet-sourced content, they can inadvertently reproduce societal biases and prejudices. This is particularly problematic when the model is used in settings where fairness and neutrality are critical.⁶³

Limitations in handling real-time data and external knowledge: GPT models are constrained by their training data and lack real-time internet access. This limitation means they cannot provide information on events or developments that occurred after their last training update. Consequently, their responses may be outdated or lack awareness of recent events, trends, and advancements.

Challenges in interpretability and transparency: Understanding the decision-making process of GPT models is complex. The 'black box' nature of these AI systems makes it difficult to investigate why a model generates a specific response, which poses challenges in ensuring accountability and trustworthiness, especially in critical applications.⁶⁴

Reliance on external validation: Due to these limitations, outputs from GPT-4 often require external validation. Users must cross-check information with reliable sources, especially for critical applications. The model's inability to self-validate or update its knowledge base in real-time means that it cannot independently correct its inaccuracies or biases.

Computational resources: One of the key challenges in utilizing OpenAI GPT models is their high computational requirements. These models necessitate substantial processing power for training, which can be a significant hurdle for organizations lacking advanced computing resources. This limitation is particularly pronounced for smaller companies or those with limited technical infrastructure. Additionally, deploying these models on edge devices poses a challenge due to the limited computational capabilities of such devices. The intensive resource demands of GPT models restrict their accessibility

and practical application, especially in settings where cutting-edge computational infrastructure is not readily available.⁶⁵

Conclusions

In conclusion, the progress in natural language processing and large language models like ChatGPT has opened up exciting opportunities for catalysis research. GPT-driven models could be valuable support in accelerating the exploration of catalytic processes. The communication highlights the potential of ChatGPT in catalysis studies, indicating additional proposals and ideas on paper related to catalysts. Overall, ChatGPT-driven models serve as powerful tools for advancing research in catalysis, enabling faster discovery and optimization of catalysts for various applications.

Conflicts of interest

The authors declare no competing financial interests.

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