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Potential to transform words to watts with large language models in battery research

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Summary

Conventional battery research often grapples with the challenge of accumulating scattered knowledge and information across countless academic resources, including papers, lectures, conferences, and more. This dispersed wealth of information spans a variety of modalities, further limiting the efficiency of literature review and methodology comparison, hindering the rapid advancement of energy storage technologies. In this perspective, we cover progress and introduce a paradigm shift catalyzed by large language models. The paradigm harnesses the power of natural language processing and artificial intelligence to enable rapid information synthesis and swift insight extraction. To illustrate the transformative potential, we present a practical demonstration of a comprehensive literature review in fast charging powered by ChatGPT, showcasing how the proposed paradigm can streamline the process of synthesizing information from a vast array of sources. This perspective underscores the profound impact of large language models on battery research, ushering in an era of efficiency and accelerated innovation in energy storage technologies.

Introduction

In the contemporary landscape of energy storage technologies, batteries assume a paramount role that transcends sectorial boundaries.¹ Their significance extends across various domains, from underpinning the proliferation of renewable energy sources^{2,3} to powering the portable electronic devices that have become ubiquitous in modern society.^{4,5} Nevertheless, as global energy demands continue their relentless ascent and environmental apprehensions intensify, the imperative for advancements in battery technology becomes increasingly pronounced.^{6,7,8} This pressing need necessitates the development of a novel research paradigm that places paramount emphasis on achieving exceptionally high levels of efficiency.

In the conventional research paradigm for battery technologies, as shown on the left in Figure 1, researchers are required to navigate a vast and dispersed

body of academic resources. These resources span multiple modalities, encompassing a myriad of articles, conferences, and lectures. Within this heterogeneous repository of information, researchers must undertake the challenging endeavor of identifying and synthesizing pertinent knowledge related to their research topics. Comprehensive literature reviews are essential not only to provide an in-depth understanding but also to stimulate innovative ideas and conceive pioneering methodologies. Afterward, the research process advances into the laboratory phase, involving experimental conduction, data collection, and result analysis.

Figure 1 Comparative illustration of conventional and LLM-transformed research paradigms

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Despite its long-standing place in the scientific tradition, the conventional research paradigm presents inherent limitations. First and foremost, the dispersed nature of the literature, spanning a multitude of sources and formats, complicates the process of consolidating relevant insights. To illustrate, there are over 300,000 entries related to batteries in the Web of Science database, with this number continually on the rise. In fact, in 2022, this count surged to nearly 40,000, signifying the rapidly expanding body of knowledge in this field. Such a sheer volume of information necessitates significant time commitments and, even so, inevitably leads to the oversight of crucial findings. Moreover, identifying the most pertinent research in this vast sea of knowledge often requires extensive manual review and expert judgment. This human-intensive approach may inadvertently limit the scope and depth of the research exploration. Furthermore, the research endeavor typically entails repeated engagement with the literature, often through multiple iterations during both the idea generation and methodology design phases, resulting in a substantial investment of time and resources. This not only hampers the pace of scientific advancement but also poses a substantial obstacle in the face of pressing global challenges that demand swift solutions.

To address these formidable challenges, the advent of multimodal artificial intelligence (AI) emerges as a promising and transformative solution. Multimodal AI systems undergo training using a diverse array of data types, including video, audio, images, and text. This multifaceted training equips AI with the capability to understand content more comprehensively and to

interpret context at greater depth. At the core of these advanced models, large language models (LLMs), such as OpenAI's ChatGPT,^{9,10,11,12,13} play pivotal roles in bridging the human-machine gap. Initially, LLMs have been characterized by their remarkable ability to understand, generate, and manipulate human language at an unprecedented scale and accuracy.^{9,10,11,12,13} These capabilities have subsequently been further extended to encompass the comprehension of various other formats of data.¹⁴ Inspired by these remarkable capabilities, LLMs have found wide-ranging applications in various academic disciplines, providing assistance in fields such as medicine for clinical decision support¹⁵; biology, as exemplified by AlphaFold's ability to deduce protein structures from amino acid sequences¹⁶; mathematics involving discovering new solutions of complex algorithmic problems¹⁷; and chemistry, for the synthesis of new compounds.¹⁸ These applications shed light on the introduction of novel research paradigms transformed by LLMs in the field of battery research, offering the promise of overcoming long-standing challenges inherent in the traditional research approach.

Transitioning to this new paradigm (refer to Figure 1), LLMs are utilized to efficiently process vast quantities of research resources and, through their language comprehension and generation capabilities, extract insights from complex and multifaceted literature sources. This newfound capability is instrumental in addressing the challenges posed by the dispersed nature of battery research literature, the difficulty in identifying pertinent information, and the time-intensive iterations required in research design. As such, leveraging LLMs in battery research (or any other area of research) has the potential to streamline the process of information extraction, thereby enabling researchers to quickly access, analyze, and apply a wealth of knowledge. By efficiently consolidating relevant information from a wide array of sources, LLMs empower researchers to expedite idea generation and methodology design, bypassing the often time-consuming and repetitive stages traditionally associated with research. Furthermore, empowered by extensive access to a rich array of research resources and their evolving cognitive prowess, LLMs can help researchers distill insights from gathered experimental data and formulate well-supported conclusions. Essentially, beyond the experimental stage that necessitates manual intervention, the incorporation of LLMs streamlines facilitation throughout every phase of the research process.

Nonetheless, it is essential to recognize that while LLMs excel in information extraction, they may not possess domain-specific knowledge, such as the

intricate details of battery technologies. This limitation can occasionally result in less-than-ideal responses to posed questions. To fully unlock the potential of this new paradigm in addressing the specific challenges of energy storage, a complementary approach is required to integrate information extraction capabilities of LLMs and the expertise of academic research resources. Such integration would create a synergistic partnership, harnessing the advantages of both LLMs and domain expertise, ultimately accelerating the advancement of innovative solutions in battery research.

To exemplify the transformative capabilities of incorporating LLMs into battery research, we demonstrate an approach in the realm of fast charging, referred to as “BatteryGPT.” Fast charging serves as a compelling example for several reasons. Firstly, it has recently gained substantial attention, driven by the burgeoning marketing and adoption of electric vehicles (EVs). The widespread adoption of EVs is instrumental in mitigating greenhouse gas emissions and enhancing energy security for nations.¹⁹ Fast-charging technology plays a pivotal role in alleviating the prevalent “range anxiety” associated with EVs. Consequently, numerous countries and regions, including the United States,¹⁹ Europe,²⁰ and China,²¹ have made significant commitments to the development of advanced electrification research aimed at enabling fast-charging solutions. As the demand for fast-charging solutions continues to escalate, the need for cutting-edge research becomes increasingly pronounced. Secondly, fast-charging technology is inherently intricate, comprising numerous technical details, intricate mechanisms, and evolving innovations.²² This complexity positions it as a highly technological field where attention to detail is paramount, making it an ideal candidate for demonstrating how LLMs can effectively address the multifaceted aspects of advanced battery research.

BatteryGPT relies on a dedicated fast-charging database sourced from a large number of publications. When prompted with user input concerning their fast-charging objectives, the BatteryGPT system seamlessly embarks on a comprehensive exploration of the expansive landscape of battery research literature. It efficiently extracts the most pertinent and current information related to fast-charging technologies. Following this information retrieval process, the LLM expertly organizes and synthesizes the wealth of knowledge, furnishing the user with a coherent and insightful summary. This summary encapsulates key findings, recent advancements, and potential methodologies pertinent to fast charging within the realm of battery technology. The concise yet powerful flow of BatteryGPT is demonstrated in Figure 2 and will be discussed in the next section.

Figure 2 Application of LLMs to an expedited research review for fast-charging technologies

Show full caption

BatteryGPT and fast charging

Fast charging stands as a pivotal requirement in battery technology that would enable a transformative leap forward with profound implications.¹⁹ Its significance lies in its ability to dramatically reduce the time required to replenish the energy stored within batteries (perhaps down to 5–10 min to go from 20% to 80% state of charge), making it an essential component of our increasingly electrified world. In the context of EVs, fast charging addresses a key concern for consumers by alleviating range anxiety, thereby accelerating the broader adoption of electric mobility.^{23,24,25} This, in turn, contributes to a significant reduction in greenhouse gas emissions and a reduced dependence on fossil fuels, fostering a more sustainable and environmentally conscious future. Beyond EVs, fast charging is pivotal for the integration of renewable energy sources into our power grids, enhancing grid stability, promoting energy sustainability, and offering a practical solution for emergency situations.^{26,27} As battery technology continues to advance, fast charging is a linchpin in ushering in a new era of convenience, environmental responsibility, and energy efficiency.

In the realm of fast-charging research, several key areas are of paramount importance.

(1)

Anode and cathode materials: the materials for both the anode and cathode impact the rate at which energy can be stored and released, directly influencing the charging speed of batteries.^{28,29,30,31,32,33,34}

(2)

Interface engineering: interface engineering ensures efficient electron and ion transport during rapid charging, reducing degradation and heat generation.^{35,36}

(3)

Microstructure optimization: fine-tuning the microstructure can improve mass transfer and overall efficiency.^{37,38,39,40,41,42,43,44,45,46,47,48}

(4)

Charging protocol design: intelligent charging protocols that take into account the specific needs and limitations of fast-charging batteries can help balance speed and battery longevity.^{49,50}

(5)

Thermal management: maintaining appropriate temperature levels during fast charging is vital to prevent overheating and thermal-induced degradation. Effective thermal management strategies are fundamental for safe and efficient fast-charging.^{51,52,53,54,55}

(6)

Manufacturing processes: developing efficient and scalable manufacturing processes is essential to bring fast-charging batteries to mass production. Ensuring consistency and quality during production is a critical research aspect.^{56,57}

From words to watts

Limited by their training corpus, general-purpose LLMs usually lack specialized knowledge required for answering professional inquiries about fast-charging technology, leading to potential inaccuracies and factual errors, commonly referred to as “hallucination.”¹³ To address this issue, one promising approach is incorporating external knowledge into prompts, a technique known as retrieval-augmented generation (RAG).⁵⁸ In essence, given a specific query, RAG first retrieves a collection of relevant knowledge from a designated source. This retrieved knowledge is then amalgamated as contextual information alongside the original query, subsequently provided to the LLM as prompt input to trigger the generation of corresponding responses. In this process, the interaction with the LLM is implemented using prompt only, and no training or fine-tuning is involved.

In fact, the RAG paradigm leverages the zero-shot learning capability of the LLM, which presents remarkable advantages in the considered scenario. Taking advantage of this framework, the integration of most up-to-date knowledge can be enabled by simply updating the knowledge database. This effectively avoids the massive computational cost for fine-tuning the LLM and mitigates the risk for retrieving irrelevant information.

Inspired by the principles of RAG, BatteryGPT is proposed to utilize LLMs to transform the landscape of fast-charging technology investigation. As

depicted in Figure 2, this innovative framework consists of two integral components: (1) the fast-charging database and (2) the question-answer (QA) engine.

Fast-charging database

The core of the fast-charging database is a central repository of knowledge extracted from an extensive collection of research articles. These articles are initially sourced through a search on the Web of Science using the keyword “fast-charging,” yielding a pool of approximately 2,200 articles. However, due to the diverse origins of these publications, web scraping techniques, conducted with proper authorization, allow for the automated gathering of only around 1,000 articles from this pool.

To enhance the resources available for BatteryGPT, this article database is further enriched by integrating the insights and expertise of researchers, leading to the inclusion of approximately 50 high-quality articles obtained through manual collection. The selection of these manually acquired articles adheres to specific criteria, including (1) the timeliness of the papers, (2) the scholarly standing of the publishers, (3) the academic reputation of authors, and (4) the quality of the literature reflected through citation metrics. A detailed list of these articles is provided in an Excel spreadsheet of fast-charging papers extracted from literature (see Data S1), with a dedicated column indicating whether the articles were downloaded automatically or manually.

This amalgamated repository, comprised of a substantial number of articles, forms the cornerstone of this research paradigm. As these articles are originally in PDF format, a subsequent step involves text parsing to extract and process the text from these documents using Python. Each paragraph within the PDF documents is parsed into text snippets, thereby ensuring that the knowledge contained within them is accessible for analysis and retrieval.

To further enhance the efficiency of knowledge retrieval, the textual data are converted into vector representations using the text embedding technique. This conversion into numerical vectors is a pivotal step, streamlining the data for computational analysis and enabling the system to rapidly retrieve and process information.

It is essential to note that, in addition to research articles, the database has the potential to incorporate a diverse array of multimodal academic resources, such as lectures and contributions from academic conferences. This expansion encompasses a variety of data formats, including traditional

text, figures, audio, video, and potentially more. This broader inclusion of data modalities offers a comprehensive and holistic perspective of the fast-charging field, ensuring that a wide spectrum of knowledge is readily available for research and analysis.

QA engine

The QA engine is crafted to interpret and respond to user-generated questions related to fast-charging technology. These posed questions are converted into vectors using the same technology as that used to construct the fast-charging database. Leveraging the vector representations of textual content, the QA engine searches the vast expanse of the fast-charging database to extract pertinent information, insights, or answers from the wealth of data stored within based on the embedding cosine similarities. Once this information is retrieved, it is amalgamated with specific formatting requirements, shaping it into a prompt for BatteryGPT. This prompt guides BatteryGPT to generate the final output, delivering concise, contextually accurate, and user-friendly answers or insights that directly address the user's questions and providing reliable references for further exploration. The algorithmic flow, along with an illustrative example, is detailed in Figure S1.

One significant challenge in this approach is the limitation of prompt length, constraining the volume of domain-specific knowledge accessible to LLMs for a given query. This limitation necessitates condensing the most pertinent and high-quality textual content within a confined input space to attain optimal output, thereby intensifying the demand for superior information retrieval. Enhancing the quality of information retrieval involves integrating various criteria such as citation analysis and author reputation into the evaluation of content quality. By incorporating these additional metrics alongside cosine similarity, the ranking of relevant content could be refined, thereby potentially enhancing Battery-GPT's output. This targeted enhancement forms a central focus for our future research endeavors.

Results of BatteryGPT

The outcomes of this transformative research paradigm for fast-charging technology, as portrayed in Figure 3, underscore its remarkable efficacy in addressing research questions and facilitating in-depth exploration of this field. This example focuses on a series of hierarchical questions that delve into various aspects of anode technology. It begins with a broad question and then follows up with more specific inquiries about structure modifications, surface modification, and electrode architecture. Each subsequent question

builds upon the previous answer, leading to a progression from broad to specific aspects. Figure 3 provides a summary of the main points for each answer for demonstration purposes. The complete and detailed answers can be found in Note S1.

Figure 3 Demonstration of generated answers using ChatGPT and BatteryGPT for various research questions

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One of the salient results is the system's ability to provide answers to research questions effectively. The vast expanse of data stored within the fast-charging database, coupled with the natural language understanding capabilities of ChatGPT, equips the system to deliver broad insights and responses to a wide array of queries, offering a comprehensive understanding of fast-charging technology.

To delve into further detail, this paradigm excels in providing precise and domain-specific responses to highly specific questions. By tapping into the domain knowledge embedded in the database, BatteryGPT demonstrates its capacity to offer detailed and contextually relevant answers that are rooted in the literature of fast-charging technology. For example, consider the question regarding surface modification technology. BatteryGPT not only lists various materials for coating but also provides specific compounds along with relevant references, rendering the answer credible and facilitating further investigation.

Moreover, BatteryGPT excels in providing answers with a remarkable degree of timeliness and precision. A noteworthy illustration is its recommendation of Li₃P for enhancing the solid-electrolyte interphase (SEI).⁵⁹ During the initial cycling of the battery, a continuous crystalline Li₃P-based SEI was spontaneously generated in situ. This process involves the precise construction of an extremely thin P nanolayer on the graphite surface, achieved through the strategic interaction of S molecules. This innovative approach involving Li₃P induces a low-solvent-coordination Li⁺ solvation structure near the inner Helmholtz plane, reducing Li⁺ desolvation barriers and enhancing SEI Li⁺ diffusion. Pouch cells equipped with this modified graphite anode achieve remarkably fast charging times of 10 and 6 min for 91.2% and 80% capacities, respectively. Notably, this represents a very recent and promising development in anode materials for fast-charging Li-ion batteries.

Another example of the prowess of BatteryGPT is its recommendation of laser-patterning technology for electrode architecture design.⁶⁰ Conventionally, the use of thick electrodes has posed challenges related to ion transport, resulting in a trade-off between power and energy density. However, by employing a laser-patterning process, it becomes possible to craft a three-dimensional graphite anode architecture characterized by vertical pore channels that serve as efficient pathways for rapid ionic transport. Such an architecture exhibits remarkable capacity retention even after numerous fast-charge cycles, significantly outperforming unpatterned electrodes. This achievement positions laser patterning as a promising avenue for the development of safe and fast-charging solutions for high-energy-density batteries.

In summary, the results underscore the versatility and proficiency of this research paradigm. While ChatGPT excels at addressing general inquiries, BatteryGPT goes a step further by drawing from domain knowledge to offer specific and expert-level responses, ultimately enriching the knowledge exploration and research experience in the realm of fast-charging technology. In comparison to traditional literature search engines like Google Scholar, the incorporation of LLMs offers significant advantages. Unlike those traditional tools that solely provide a list of related articles, LLMs can comprehend and summarize the content into insightful categories, thus enabling more organized and hierarchical research.

Outlook and perspectives

As exemplified by the capabilities of BatteryGPT, this innovative research paradigm powered by LLMs offers a profound transformation in the domain of fast-charging technology research. The results we have witnessed underscore the paradigm's exceptional proficiency in enabling rapid information synthesis and swift insight extraction. These insights can be retrieved in an organized manner, making the research process more efficient and streamlined. Another key strength of this paradigm is its adaptability and capacity for continuous growth. The fast-charging database can be dynamically updated with new literature, ensuring that the generated information remains current and aligned with the latest research. Furthermore, the system not only provides answers but also furnishes reliable references for further exploration, enriching the user experience and promoting in-depth research. This feature can be further enhanced by ranking the reliability of references using meta information, such as the

number of citations and the reputation of publishers. This will be the focus of our future work.

In a broader perspective, this innovative research paradigm, transformed by LLMs, holds the potential to propel innovation across a spectrum of new energy research domains. Its efficiency in knowledge retrieval and the generation of contextually accurate responses transcends the confines of fast-charging technology, serving as a template for reshaping the research landscape in various disciplines.

Furthermore, with the rapid advancements in transformative technologies, including LLMs and other AI tools, the application scope of these evolved paradigms extends well beyond traditional text-based outputs. Their inherent adaptability empowers them to produce outputs in diverse formats, spanning from code scripts to audio narrations and even video presentations. This adaptability caters to a wide array of research scenarios and diverse research needs.

Figure 4 outlines some of the promising perspectives where LLM-transformed paradigms can be leveraged, marking a pivotal shift in the way we approach research in an ever-evolving landscape.

Figure 4 Perspective of LLMs in battery research

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Research review

(1)

Content comprehension: LLMs can be employed to swiftly comprehend extensive volumes of research resources, assisting in the synthesis of complex content.

(2)

Related work summary: with unrestricted access to a vast repository of research resources, these systems possess the capability to autonomously produce comprehensive summaries of related work. This approach not only expedites the literature review process but also offers a more holistic and insightful perspective.

(3)

Research trend analysis: LLMs are invaluable for identifying emerging trends in research topics, offering researchers insights into the evolving landscape of their field.

Methodology design

(1)

Method recommendation: leveraging the wealth of expertise within research resources, LLMs can offer guidance on the most relevant, effective, or commonly employed research approaches within a given field or topic.

(2)

Troubleshooting current methods: these paradigms are adept at diagnosing issues in current research methods and providing solutions to overcome them.

(3)

Method optimization: after troubleshooting, LLMs can offer relevant solutions by drawing upon similar knowledge from their database, thereby enhancing overall efficiency and effectiveness.

Result analysis

(1)

Data interpretation and summarization: LLMs can aid in the interpretation of complex research data, offering valuable insights and facilitating meaningful conclusions.

(2)

Comparative analysis: researchers can employ these systems to conduct comparative analyses, assisting in drawing comparisons between research outcomes.

(3)

Data visualization: LLMs have the capability to generate code snippets to assist in crafting data visualizations, enabling the presentation of research outcomes in a clear, visually engaging, and comprehensible manner.

Academic communication

(1)

Presentation assistance: LLMs can assist in creating compelling presentations, ensuring clear and impactful communication of research findings.

(2)

Lectures and interactive reports: these paradigms can be harnessed to generate lecture materials and interactive reports, fostering engaging and informative academic communication.

In essence, the adaptability and transformative potential of LLM-transformed paradigms are not limited to any single field but extend across a wide spectrum of research scenarios and formats. As these systems continue to evolve, they hold the promise of streamlining research, enhancing innovation, and facilitating effective communication within the academic and research communities.

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Author contributions

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Declaration of interests

The authors declare no competing interests.

Declaration of generative AI and AI-assisted technologies in the writing process

During the preparation of this work, the authors used ChatGPT in order to polish the draft. After using this tool, the authors reviewed and edited the content as needed and take full responsibility for the content of the publication.