

Emerging Trends in Chat GPT for Computational Material Science.

Dr. Alla Srivani¹, Dr. Gurram VeeraRaghavaiah², Nagaraju Dasari³, Srinivasa Rao Bogireddy⁴

Professor, Vasireddy Venkatadri Institute of Technology, Guntur Dt AP, India

Principal & HOD of MCA Department, PAS College, Guntur Dt, AP, India

Principal Engineer, Navy Federal Credit Union, 820 Follin Lane SE, Vienna, VA, USA

Sr. Software Engineer, Horizon systems Inc, 46090 Lake Center Plaza, Unit 209 Sterling, VA, USA

Abstract: In computational materials science, the primary step is typically the creation of a model or structure. For example, in Density Functional Theory DFT, the initial step is the creation of an appropriate molecular or crystalline structure. To begin, one can request Chat GPT for assistance in constructing an atomic structure for a lithium metal surface, which is one of the most important surfaces in the battery and energy sciences. To construct a lithium slab, one can attempt to query Chat GPT for the ability to generate a Customer Identification File for the surface. Visualizing the output Identification File, one can observe that the structure is not a slab per se, but rather a unit cell containing one atom. The Identification File Identification File CIF file can be further expanded to a maximum of 16 atoms by asking Chat GPT: "Can you expand Identification File CIF for lithium slab to 16 atoms?" The resulting output is a box containing 16 random atoms.

Keywords: Computational Material Science, DFT, chat GPT, Atomic structure

Introduction

Chat GPT has recently become a widely discussed artificial intelligence tool, capable of "chatting" with humans. It can be used to complete a variety of tasks, including essay writing, coding, composition, painting, and more. While the role of Chat GPT has been widely discussed in aiding in literature review and language editing, its potential applications in computational materials science remain to be explored. In this article, we will briefly outline three aspects of Chat GPT that could potentially be used in computational materials science, such as building structures, writing code for particular scientific software, and creating data visualization scripts. While Chat GPT may make some basic errors when attempting to complete general tasks, it is able to learn from our language when communicating with us. We should be aware of issues such as consistency output, hidden mistakes, and ethical considerations. We hope this perspective will encourage further exploration of Chat GPT's potential applications in materials science. Reason for choosing this topic in materials science and engineering, Chat GPT is all about coming up with new research concepts and ideas. AI models can look at existing data and studies to spot any gaps in understanding and come up with new research

ideas.

Chat GPT is an effective tool for facilitating comprehension by providing students with questions and prompts to help them gain a better understanding of the literature being read. Additionally, the model can be utilized to encourage critical thinking skills, such as analyzing, evaluating, and synthesizing information. Simulated scenarios or debate can also be created using Chat GPT to help students develop their critical and logical thinking skills.

Objectives: Chat GPT has shown some promising results in answering physics problems that are conceptual in nature. When it comes to high-school-level physics, Chat GPT seems to be able to solve most school physics questions, including basic mathematical calculations. Chat GPT was able to answer most of the multiple-choice questions correctly in an introductory-level college astrophysics exam, scoring highly. It even provided explanation. Writing a literature review with Chat GPT can make the research process much easier. With a step-wise approach, researchers can take advantage of Chat GPT's features to collect data, create content, and improve their literature review.

Methods

It is not possible to ask chat bots, even high-performance bots such as Chat GPT, simply to search and extract information from the entire text of a paper. To refine the technique, Polak asked the bots to review the text sentence by sentence and determine whether each sentence contained relevant information or not—a process that reduced the paper to one or two critical sentences. He then requested the bots to submit the information in the form of a table. At this point, a human researcher could examine the table and the sentences to verify their accuracy and relevance. The technique achieved an accuracy rate of approximately 90%. The researchers were able to extract information from a series of papers to generate a database on critical cooling rates of metallic glasses.

Chat GPT can help speed up the process of research ideation, implementation, and validation. For instance, it can show you all the research methods that are related to the questions and problem area. Plus, it can give you a ranking of the methods based on how effective they are. The experts said that Chat GPT can help you get the main points and the gist of

in no time. The experts said Chat GPT were especially useful for writing research reviews.

Results

Industrially chat GPT is used in Pharmaceuticals for Researching and developing new medicines has become increasingly time-consuming. Wealth management. Staffing shortages have handicapped multiple industries, including finance and Automotive.

In recent years, artificial intelligence (AI) and machine learning have changed the landscape of scientific research. Chat bot technology has come along way in recent years, especially with his Chat GPT being developed into a notable AI language model. This comprehensive overview explores Chat GPT's background, applications, key challenges, and future directions. We will first examine its origins, development, and underlying technology, and then examine its wide range of applications in industries such as customer service, health care, and education. We also highlight key challenges facing Chat GPT, such as ethical concerns, data distortion,

and security issues, and discuss possible mitigation strategies. Finally, we envision the future of Chat GPT by exploring further areas of Research & Development R&D, focusing on integration with other technologies, enhancing human-AI interaction, bridging the digital divide. This review provides valuable insights for researchers, developers, and stakeholders interested in the evolving landscape of AI-driven conversational agents. This study explores the many ways Chat GPT has revolutionized scientific research, from data processing and hypothesis generation to collaboration and outreach.

Discussion

This Research Paper examines the potential challenges and ethical concern associated with his use of Chat GPT in his research, and highlights the importance of striking a balance between AI innovation and human expertise increase. This paper introduces some ethical issues in the existing computing space and how Chat GPT can challenge this notion. This work also includes some biases and limitations of Chat GPT. Despite some controversy and ethical concerns, it is worth noting that Chat GPT has attracted the attention of academia, research and industry in a very short period of time.

References:

- [1] S.S.Biswas, Potential use of chat GPT in global warming Ann. Biomed. Eng. (2023), pp. 1
S.S.Biswas, Role of chat GPT in public health Ann. Biomed. Eng. (2023),
- [2] R.W.McGee, Annie Chan: Three Short Stories Written with Chat GPT (2023)
- [3] R.W.McGee, Is chat GPT biased against conservatives? An empirical study Empir. Stud. (2023)
- [4] A.Mathew, Is artificial intelligence a world changer? A case study of OpenAI's chat GPT, Recent Prog. Sci. Technol., 5 (2023), pp. 35-42
- [5] M. J.Ali, A .Djalilian, Readership awareness series – paper 4: chatbots and Chat GPT-ethical considerations in scientific publications, Seminars in Ophthalmology, Taylor & Francis (2023, March), pp. 1-2