

Extracting Accurate Materials Data from Research Papers with Conversational Language Models and Prompt Engineering - Example of ChatGPT

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There has been a growing effort to replace hand extraction of data from research papers with automated data extraction based on natural language processing (NLP), language models (LMs), and recently, large language models (LLMs). Although these methods enable efficient extraction of data from large sets of research papers, they require a significant amount of up-front effort, expertise, and coding. In this work we propose the **ChatExtract** method that can fully automate very accurate data extraction with essentially no initial effort or background using an advanced conversational LLM (or AI). **ChatExtract** consists of a set of engineered prompts applied to a conversational LLM that both identify sentences with data, extract data, and assure its correctness through a series of follow-up questions. These follow-up questions address a critical challenge associated with LLMs - their tendency to provide factually inaccurate responses. **ChatExtract** can be applied with any conversational LLMs and yields very high quality data extraction. In tests on materials data we find precision and recall both over 90% from the best conversational LLMs, likely rivaling or exceeding human accuracy in many cases. We demonstrate that the exceptional performance is enabled by the information retention in a conversational model combined with purposeful redundancy and introducing uncertainty through follow-up prompts. These results suggest that approaches similar to **ChatExtract**, due to their simplicity, transferability and accuracy are likely to replace other methods of data extraction in the near future.

INTRODUCTION: Automated data extraction is increasingly used in to develop databases in materials science and other fields [1]. Many databases have been created using natural language processing (NLP) and language models (LMs) [2–24]. Recently, the emergence of large language models (LLMs) [25–29] has enabled significantly greater ability to extract complex data accurately [30, 31].

These automated methods require a certain amount of effort to set up, either preparing parsing rules, fine-tuning or re-training a model, or some combination of both, which specializes them to perform a specific task. With the emergence of highly capable, pretrained for general tasks, conversational LLMs (or AIs) such as **ChatGPT**, there are opportunities for significantly improved information extraction that require almost no initial effort. These opportunities are enabled by harnessing the high general language abilities of conversational LLMs, their inherent capability to perform zero-shot classification, accurate word references identification, and information retention capabilities for text within a conversation. These capabilities, combined with *prompt engineering* i.e. *designing questions and instructions (prompts) to improve the quality of results, can result in accurate data extraction without the need for fine-tuning of the model, extensive coding, or significant knowledge about the property for which the data is to be extracted*. In this paper we demonstrate that using conversational LLMs such as **ChatGPT** in a zero-shot fashion with a well-engineered set of prompts can be a very flexible, accurate and efficient

method of extraction of materials properties in the form of *Material*, *Value*, *Unit*. We were able to minimize the shortcomings of these conversational models - their factual incorrectness and hallucinations, and achieve perfect 100% precision and very a high recall of over 90%. This is achieved by identifying relevant sentences, asking the model to extract details about the presented data and then scrutinizing it in a form of a conversation by asking a series of follow-up questions that suggest uncertainty of the extracted information and introduce redundancy. We call this method **ChatExtract** and provide a simple to implement workflow for a fully automated approach to data extraction. The method works in a zero-shot fashion, i.e. requires no fine-tuning or any prior set-up. The prompt engineering proposed here is expected to work for all *Material*, *Value*, *Unit* data extraction tasks. For different types of data extraction this prompt engineering will likely need to be modified, but we believe that the general workflow of well-engineered prompts applied within an information retaining conversational model and redundant questioning of the extracted information will provide an effective and efficient approach to many types of information extraction.

The **ChatExtract** method is largely independent of the conversational LLM used and is expected to improve as the LLMs improve. Therefore, the astonishing rate of LLM improvement is likely to further support the adoption of **ChatExtract**-like approaches to data extraction. Prompt engineering has now become a standard practice in the field of image generation [32–34] to ensure high quality results. A parallel situation may soon occur for data extraction. Specifically, a workflow such as that presented here with **ChatExtract**, which includes prompt engineering utilized in a conversational set of prompts

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with follow-up questions, may become a method of choice to obtain high quality data extraction results from LLMs.

RESULTS AND DISCUSSION: Figure 1 shows a simplified workflow illustrating our approach, while the fully detailed workflow, including all of the necessary steps is shown in Fig. 2. Figure 2 provides all the necessary information on how the process of data extraction is conducted so here we only summarize the key ideas behind this workflow. The initial step is preparing the data and involves gathering papers, removing html/xml syntax and dividing into sentences. This is a straightforward task, more on which can be found in [31]. Next, a first prompt is given to the model. This first prompt is meant to provide information whether the sentence is relevant at all for further analysis, i.e. whether it contains the data for the property in question (value and units). This classification is crucial as the ratio of relevant to irrelevant sentences is typically about 1:100. Therefore elimination of irrelevant sentences is a priority in the first step. We then first expand the text we operate on to a passage consisting of three sentences: the paper’s *title*, the sentence *preceding* the positively classified sentence from the previous prompt, and the *positive sentence* itself. This expansion is primarily useful for making sure we include text with the material’s name. The relevant texts vary in their structure and we found it necessary to use different strategies for data extraction for those sentences that contain a single value and those sentences that contain multiple values. Therefore, the next prompt aims at determining whether there are multiple data points included in a given sentence, and based on that answer one of two paths is taken, different for a *single-valued*, and *multi-valued* sentences. Next, the text is analyzed. For a single-valued text, we directly ask questions about the data in the text, asking separately for the value, its unit, and the material’s name. It is important to explicitly allow for an option of a negative answer, reducing the chance that the model provides an answer even though not enough data is provided, limiting the possibility of hallucinating the data. If a negative answer is given to any of the questions, the text is discarded. For the case of a multi-valued sentence, instead of directly asking for data, we ask the model to provide structured data in a form of a table. This, while efficient, is more likely to produce factually incorrect data, even if explicitly allowing negative responses. Therefore, we scrutinize each field in the provided table by asking follow-up questions whether the data and its referencing is really included in the provided text. Again, we explicitly allow for a negative answer and, importantly, plant a seed of doubt that it is possible that extracted table may contain some inaccuracies. Similarly as before, if any of the answers are negative, we discard the sentence. It is important to notice that despite the capability of the conversational model to retain information throughout the conversation, we repetitively provide the text with each prompt. This repetition helps in maintaining all of the details about the text that is being analyzed, as the model tends to

pay less attention to finer details the longer the conversation is carried. The conversational aspect and information retention improves the quality of the answers and reinforces the format of short structured answers and possibility of negative responses. The importance of the information retention in a conversation is proven later in the text by repeating the exercise but with a new conversation started for each prompt, in which cases both precision and recall are significantly lowered. It is also worth noticing that we enforce a strictly *Yes* or *No* format of answers for follow up questions, which enables automatizing of the process. Otherwise the model tends to answer in full sentences which are hard to automatically analyze.

The prompts described in the flowchart (Fig. 2) are engineered by optimizing the accuracy of the responses through trial and error on various properties of varying complexity. Obviously, we have not exhausted all options, and it is likely that further optimization is possible. We have, however, noticed that contrary to intuition, providing more information about the property in the prompt usually results in worse outcomes, and we believe that the prompts proposed here are a reliable and transferable initial set. We have investigated the performance of this approach on the property bulk modulus. Our test data is taken from a large body of sentences extracted from hundreds of papers with bulk modulus data. We randomly selected 100 relevant sentences (containing data) and 100 irrelevant sentences (not containing data). In these 100 sentences with data, there were a total of 175 data points. We investigated the performance of multiple versions of ChatGPT models (see Tab. I). In the first classification step, for the best performing models, all 100 of the relevant sentences are properly determined as relevant (100% recall), and all remaining 100 are correctly determined to be irrelevant (100% precision). We then follow the approach as described above and in Fig. 2, and divide the results into categories by type of text: single-valued and multi-valued. These results are summarized in Tab. I.

In order to classify a datapoint as a successful and accurate extraction, we required that the unit was identical to that in the text, the value was identical to that in the text (with or without uncertainty, if presented in the text), and the material name was the same as in the text and allowed for a unique identification of the system. In the case of our bulk modulus dataset multi-valued sentences also outnumbered single-valued cases, with 36% being single-valued and 64% being multi-valued. Our follow-up question approach proved to be very successful for the best conversational model (ChatGPT - legacy (text-davinci-002-paid)). Overall, the model averaged to a performance yielding 100% precision at 90.3% recall, which is very impressive for a zero-shot approach that does not involve any fine-tuning. These values are close to what we assume a human would achieve, and maybe even higher if the human is not an expert in the field. Single-valued sentences tend to be extracted

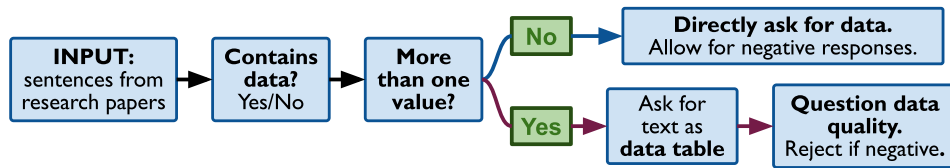


FIG. 1. A simplified flowchart describing the process of extracting structured data using a conversational large language model. Only the key ideas for each of the steps are shown, with the fully detailed workflow presented in Fig. 2

with slightly higher recall (98.1%) compared to multi-valued sentences with a recall of 87%. The API version of ChatGPT, a model called `gpt-3.5-turbo-0301` has also been evaluated, but yielded a worse, although still impressive, result. Precision remained largely unaffected, proving our follow-up question approach to be successful in assuring factually correct data. However, the recall was impacted by the change of model, lowering overall to 75.1%.

Its important to understand what aspects of ChatGPT are being used in ChatExtract that make this approach so successful. We believe that there are three core features. The first one is the set of prompts and follow-up questions, engineered in a way to verify the extracted data. By their redundancy and engineering them in a way that introduces the possibility of uncertainty about the previously extracted data, they substantially improve the factual correctness, and therefore, precision of the extracted information. Enforcing the structure of the response helps to easily automate the process. The second one is the conversational aspect, in which information about previous prompts and answers is retained. This allows the follow-up questions to relate to the entirety of the conversation, including the model’s previous responses. Lastly, the quality of the model itself is important, as it seems that the modern ChatGPT models are more capable than non-conversational GPT-3.5 based LLMs. Good statistics as a result of our follow-up questions approach are not a proof that the approach works or is necessary. They also do not prove that information retention provided by the conversational model is necessary or that the conversational model is an improvement over regular LLMs. In order to prove all three points we repeated the exercise three times: *no follow-up*, i.e. for the best performing model (ChatGPT - legacy (text-davinci-002-render-paid)) but without any follow up questions (directly asking for structured data only, in the same manner as before, using third prompt in the multi-value branch in Fig. 2); *no chat* i.e. with best performing model but starting new conversation each time; and *GPT-3.5 chat-like* i.e. simulating a conversation in regular non-conversational GPT-3.5 text-davinci-003 (by relaying the entire content of the conversation from the beginning in each prompt, including the model’s answers). The results of this exercise are summarized in Tab. I. Removing follow-up questions reduces the precision to 80.2% and recall to 88.0%. Removing the conversational aspect and asso-

ciated information retention reduces the recall and precision to 90.0% and 56.6% respectively. Using a non-conversational model in a conversational fashion with follow-up questions resulting in a relatively high precision (due to the follow-up questions) of 89.3% but a low recall of 61.7%. All of these tests result in a noticeably lower statistics than our ChatExtract approach, which includes well-engineered follow-up questions in a fully conversational fashion, i.e. where prompts and their responses are properly separated within the model. Overall these results show that using state-of-the-art conversational AI with a ChatExtract workflow such as the one presented in Fig. 2 is a viable and an accurate method for materials data extraction that does not require fine-tuning or extensive coding. These results suggest that this approach is likely to replace other methods of data extraction from scientific texts in the future.

As a final detail, it is important to remember that at the moment of writing this paper, the ChatGPT model is a closed model. In particular, the most accurate model according to our assessment presented here - ChatGPT legacy (text-davinci-002-render-paid) is accessible through website interface only and provides no op-

	Single-valued	Double-valued	Overall
ChatGPT - legacy (text-davinci-002-render-paid)	P=100% R=98.1%	P=100% R=87.0%	P=100% R=90.3%
ChatGPT - API (gpt-3.5-turbo-0301)	P=95.8% R=88.5%	P=100% R=69.1%	P=98.5% R=74.8%
ChatGPT (no follow-up) (text-davinci-002-render-paid)	P=59.7% R=81.1%	P=92.5% R=90.2%	P=80.2% R=88.0%
ChatGPT (no chat) (text-davinci-002-render-paid)	P=98.0% R=94.2%	P=83.3% R=40.7%	P=90.0% R=56.6%
GPT 3.5 (chat-like) (text-davinci-003)	P=97.2% R=67.3%	P=85.9% R=59.3%	P=89.3% R=61.7%

TABLE I. Precision (P) and recall (R) for different types of text passages containing data. Bold font represents models used within the full ChatExtract workflow, while the remaining three demonstrate the importance of redundant follow-up questioning (no follow-up), conversational information retention aspect (no chat), and using a conversational LLM over a regular LLM (GPT-3.5 chat-like).

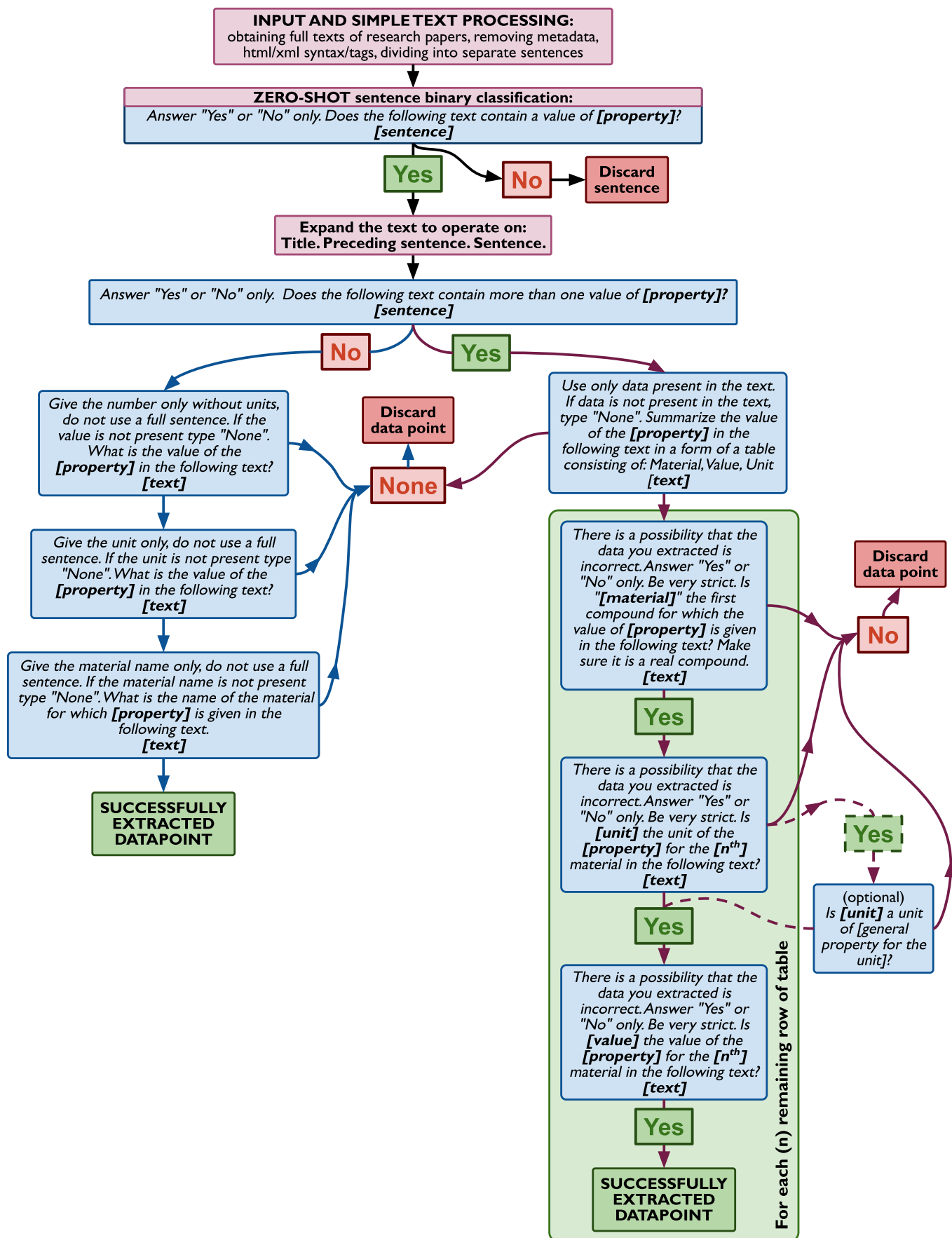


FIG. 2. A flowchart describing the process of extracting structured data using a conversational large language model. Blue boxes represent prompts given to the model, grey boxes are instructions to the user, "Yes", "No", and "None" boxes are model's responses.

tions for any parameter choice. Therefore, there is a certain degree of randomness to the answers that it provides. During our research it performed very consistently most of the time. For example, asking the first prompt we use for general classification multiple times always resulted in the same result. However, in rare cases, asking the exact same question multiple time eventually resulted in a different answer, in particular in cases where the answer to the questions may be ambiguous. This difference would usually have no consequences as the problem would be fixed in subsequent follow-up questions. The API version of ChatGPT `gpt-3.5-turbo-0301` has a "temperature" parameter, which when set to zero (as we did for our tests) improves the consistency and reliability of the responses. It is also reasonable to assume that in future releases of ChatGPT and other conversational LLMs, some tuning will be available to the user (akin to the "temperature" parameter) which could eliminate these issues by forcing the LLM to follow the instructions in the prompt more strictly and provide consistent repeatable results. Future releases will likely also provide an API which will make the proposed extraction method straightforward to apply on large scale problems.

To further demonstrate that this approach is effective we selected additional 20 sentences containing 30 values of critical cooling rates from our previously curated database [31], and put them through our data extraction process. No changes were made to the approach except for simply changing the name of the property from *bulk modulus* to *critical cooling rate*. The results were very similar to the bulk modulus data. In fact, all but one value were extracted, and all were extracted correctly, yielding, once again, perfect 100% precision and a very high recall of almost 97%.

The assessment in this work is limited due to the fact that at the moment of writing this paper the most accurate LLM for our tests is ChatGPT - legacy (`text-davinci-002-render-paid`), which is only accessible through a website interface, and does not allow for automated access. Therefore all of the assessments presented here for this model have been done by manually inputting the prompts and sentences into the chat. It is, however, crucial to be able to assess these quickly emerging methods for their suitability in materials science applications as soon as possible, so that once they

are released in a form allowing for automated usage, researchers are ready to take advantage of their full capabilities.

CONCLUSIONS: This paper demonstrates that conversational LLMs such as ChatGPT, with proper prompt engineering and a series of follow-up questions, such as the ChatExtract approach presented here, are capable of providing high quality materials data extracted from research texts with no additional fine-tuning, extensive code development or deep knowledge about the property for which the data is extracted. We present such a series of well-engineered prompts and follow-up questions in this paper and demonstrate its effectiveness resulting in a best performance of 100% precision at 90.3% recall on our test set of bulk modulus data, which is comparable to or surpasses human performance. We show that the success of the ChatExtract method lays in the information retention within the conversation and purposeful redundancy with introduction of uncertainty, by comparing the results if these aspects are removed. The high quality of the extracted data and the simplicity of the approach suggests that approaches similar to ChatExtract offer an opportunity to replace previous, more labor intensive, methods.

METHOD: The results of the web-based ChatGPT were obtained between Feb. 13th and Mar. 14th, 2023 (dates are included to indicate the version), through an account with a *Plus* subscription. For ChatGPT API (`gpt-3.5-turbo-0301`) and GPT-3.5 (`text-davinci-003`), default parameters were used, except for temperature frequency and presence penalties, which have been set to zero.

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DATA AVAILABILITY: The data used in the assessment of the model together with transcripts of all conversations with the models and their results is available on figshare [35]: <https://doi.org/10.6084/m9.figshare.22213747>.

CONTRIBUTIONS: M. P. P. conceived the study, performed the modeling, tests and prepared/analyzed the results, D. M. guided and supervised the research. Writing of the manuscript was done by M. P. P. and D. M..

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