SciQAG: A Framework for Auto-Generated Science Question Answering Dataset with Fine-grained Evaluation

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Abstract

We introduce SciQAG, a novel framework for automatically generating high-quality science question-answer pairs from a large corpus of scientific literature based on large language models (LLMs). SciQAG consists of a QA generator and a OA evaluator, which work together to extract diverse and research-level questions and answers from scientific papers. Utilizing this framework, we construct a large-scale, high-quality, open-ended science QA dataset containing 188,042 QA pairs extracted from 22,743 scientific papers across 24 scientific domains. We also introduce SciQAG-24D, a new benchmark task designed to evaluate the science question-answering ability of LLMs. Extensive experiments demonstrate that finetuning LLMs on the SciOAG dataset significantly improves their performance on both open-ended question answering and scientific tasks. To foster research and collaboration, we make the datasets, models, and evaluation codes publicly available, contributing to the advancement of science question answering and developing more interpretable and reasoningcapable AI systems.

1 Introduction

Question-answering (QA) datasets have been instrumental in advancing natural language processing (NLP) research by enabling the development of models that can understand and reason about textual information. These datasets encompass various domains and question types, such as reading comprehension (Hermann et al., 2015), open-domain QA (Chen et al., 2017; Longpre et al., 2021), and visual QA (Schwenk et al., 2022; Masry et al., 2022). They serve as benchmarks for evaluating

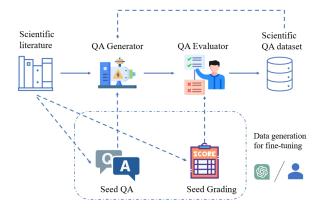


Figure 1: The SciQAG framework for generating science QA from the scientific literature. The dashed line represents optional fine-tuning.

the performance of QA systems and drive the creation of more sophisticated models (Chen et al., 2017; Rajpurkar et al., 2016). Among these, science QA datasets such as SciQ (Welbl et al., 2017) and SciencQA (Saikh et al., 2022) have garnered significant attention due to their potential to assess models' ability to comprehend and apply scientific knowledge (Clark et al., 2018; Mihaylov et al., 2018). The importance of these datasets lies not only in their capacity to test models' understanding of scientific concepts but also in their ability to evaluate the models' reasoning capabilities when dealing with complex relationships and drawing conclusions based on experimental evidence.

The advent of large language models (LLMs) like GPT-4 (OpenAI et al., 2023), LLaMA-3 (Touvron et al., 2023b), PaLM (Chowdhery et al., 2022), marks a significant milestone in the pursuit of general artificial intelligence. These models have proven instrumental in various aspects, includ-

ing generation, annotation, and paraphrasing (Yoo et al., 2021; Xie et al., 2024; Sahu et al., 2022; Xie et al., 2023b; Wang et al., 2023; Tang et al., 2023). Besides general applications, this trend has permeated the natural sciences, giving rise to domainspecific models like BioBERT (Lee et al., 2020), Med-PALM (Singhal et al., 2022), and Galactica (Taylor et al., 2022). While these models may not always necessitate pre-training from scratch, it often involves fine-tuning on domain-specific data. QA pairs are essential for fine-tuning and evaluating LLMs (Kamalloo et al., 2023; Rasool et al., 2024), particularly when domain-specific questionanswering capabilities are desired. For example, (Zhang et al., 2024a) fine-tuning data comprises 7M instruction tuning QA pairs, with the objective of instruction fine-tuning often being causal language modeling in GPT-based scientific LLMs (Zhang et al., 2024b). As such, the development of more comprehensive science QA datasets and related evaluation methods is a practical necessity for advancing scientific LLMs.

Despite the progress made with existing science QA datasets, several challenges persist. First, these datasets often lack variety in question forms, with most being multiple-choice questions (MCQ). Although the performance of MCQs is established by exact match and conclusions obtained from such evaluation tend to be more robust (Subramanian et al., 2024), they inadequately test the language and logical reasoning capabilities of LLMs, necessitating more challenging QA benchmarks. Second, the content of these datasets is primarily sourced from textbooks, resulting in an insufficient difficulty level to assess the high-level knowledge retention of LLMs in real-world academic research or industrial production settings. Third, the creation of these benchmarks often relies on crowd-sourcing or expert-driven approaches, which can be costly (Lee et al., 2023a; Xie et al., 2023c) due to the need for specialized skills (Xie et al., 2023a; Ye et al., 2024). Addressing these challenges is crucial for developing robust and comprehensive QA datasets that can more accurately evaluate the capabilities of scientific LLMs.

To tackle these challenges, we focus on the task of open-ended, closed-book science QA in this paper. Open-ended questions do not have predetermined or fixed answers, while closed-book indicates that no external knowledge or context is provided with the question (Roberts et al., 2020).

We introduce Automatic Generation of Science Question Answering (SciQAG), a framework for automatically generating QA pairs from scientific articles (see Figure 1). SciQAG comprises two main components: a QA generator and a QA evaluator. The QA generator leverages LLMs to extract relevant information from scientific papers and generate diverse question-answer pairs while the QA evaluator assesses or filters the generated QA pairs. By applying SciQAG to a large corpus of scientific papers, we constructed a high-quality science QA dataset, SciQAG-24D, consisting of 188,042 QA pairs. We compared the zero-shot performance of several LLMs on the SciQAG-24D test set and explored fine-tuning impacts of the training set on various datasets, including unseen QA pairs, SciQ (Welbl et al., 2017), and scientific tasks. The results demonstrate that incorporating science QA data during fine-tuning significantly enhances the model's ability to understand and apply scientific knowledge, improving performance on various scientific tasks. These findings underscore the value of the SciQAG-24D dataset and highlight the potential of scientific LLMs in advancing scientific research and problem-solving.

2 Related Work

2.1 Science QA benchmarks

Science QA benchmarks, which typically consist of questions and answers from scientific literature, textbooks, or domain experts, play a crucial role in evaluating the performance of QA systems in scientific domains. Table 1 provides a comparison of several popular science QA benchmarks, highlighting the prevalence of manually collected elementarylevel multiple-choice questions Notable examples includes the work of Welbl et al. (2017), who proposed a novel approach to assist crowd workers in generating MCQs with answers from relevant passages. Lu et al. (2022) compiled a multi-modal multiple-choice QA dataset from elementary and high school science curricula, emphasizing the evaluation of model reasoning skills. In the biomedical domain, Jin et al. (2019) produced a QA dataset based on PubMed article abstracts, focusing on reasoning beyond factoid answer extraction, but limited to yes, no, or maybe answers. However, most previous open-ended long-form QA datasets on scientific literature are limited to domains like AI (Lee et al., 2023b; Dasigi et al., 2021) or biomed-

Dataset	Size	Method	Q-type	Difficulty
SciQ (Welbl et al., 2017)	13,679	Manual	MCQ	Element - college
ScienceQA (Saikh et al., 2022)	21,208	Manual	MCQ	Element - high
OpenBookQA (Mihaylov et al., 2018)	5,957	Manual	MCQ	Element
ARC (Clark et al., 2018)	7,787	Manual	MCQ	Element
MMLU (Hendrycks et al., 2020)	15,908	Manual	MCQ	Element - profession
SciQA (Auer et al., 2023)	2,565	Automated	Open-ended	Profession

Table 1: Overview of several popular science QA benchmark datasets, including their size, construction method, question type, and difficulty level.

ical (Otegi et al., 2022; Jin et al., 2021), leaving room for the development of more comprehensive and diverse science QA benchmarks.

2.2 Automatic QA generation

Automatic question generation has been explored in various contexts, with a primary focus on educational applications. Early methods utilized syntactic transformation templates (Mitkov et al., 2003; Heilman and Smith, 2010)to transform text into questions. Pandya and Bhatt (2021) established a taxonomy for human-generated QA datasets and evaluation strategies for comparing modelgenerated answers with reference answers. However, current automatic question-generation methods typically rely on predefined answers (Mulla and Gharpure, 2023). For example, Virani et al. (2023) introduced a versatile Question Answer Generation (QAG) system, adaptable to various question types and domains, but it still requires predefined answers for question generation. Recently, Auer et al. (2023) used a rule-based method to automatically build SciQA for scholarly knowledge; but this approach relies on an existing knowledge graph. In contrast, the approach presented in this paper aims to generate high-quality open-ended QA pairs from scientific texts without relying on manually curated answers, thus addressing a gap in current literature.

2.3 Evaluation metrics for open-ended QA

Evaluating the quality of long-form generated text, such as open-ended QA pairs, is a challenging task due to the subjective nature of the assessment (Das et al., 2021). Traditional evaluation metrics, including BLEU (Papineni et al., 2002), ROUGE (Lin, 2004), METEOR (Banerjee and Lavie, 2005a), and F1 (Rajpurkar et al., 2016), rely on *n*-gram between the generated text and a reference text. More recent methods, such as BERTScore (Zhang et al., 2020), sentence mover similarity (Clark et al., 2019), and

MAUVE (Pillutla et al., 2021) eliminate the need for *n*-gram similarities, but still require reference texts (Chen et al., 2019). Min et al. (2023) propose an alternative approach that evaluates the factuality of long-form generated text by breaking it down into atomic facts and computing the percentage of atomic facts supported by a reliable knowledge source. The application of large language models (LLMs) to evaluate the quality of generated science QA datasets (Song et al., 2023) has also shown promise. Building upon these advancements, this paper adopts a multi-perspective approach using LLMs to evaluate the quality of open-ended QA pairs, contributing to the development of more comprehensive evaluation metrics for science QA.

3 SciQAG framework

We propose a cost-effective framework to generating closed-book QA pairs focusing on scientific knowledge from the literature at scale, called SciQAG. The main idea is to train a generator to convert full-text scientific papers into QA pairs and use an evaluator to filter out those that do not meet quality standards.

3.1 QA generator

The task is defined as follows: given seed input texts T, for each input text t, the generator should firstly generate 15 keywords k that capture the most important terms and concepts in the text, then generate a set $S = \{(q_i, a_i)\}_{i=1}^n$ focusing on the generated keywords k, where $\forall i \in \{1, ..., 10\}, q_i$ is the question and a_i is the answer to q_i . To generate S, one should learn a generator $G(S|T;\theta)$ with θ the model parameters. Thus, given a new input text \hat{t} , following $G(S|T;\theta)$, one can directly generate a \hat{S} consisting of QA pairs (by firstly generating 15 keywords to guide the QA generation).

We designed an effective prompt for LLM to generate QA pairs with detailed information ex-

tracted from scientific papers. Since our final generated QA dataset is intended to be closed-book, implying that models trained on our dataset will not have access to background knowledge during either training or inference, we also give guidelines to ensure that the generated QA do not depend on or reference the content in the original paper (see Appendix D for prompts).

For the dataset generation in this study, we chose to fine-tune an open-source LLM as the generator to balance performance and cost (see Section 4.2). However, users of this framework can select any open-source or closed-source LLM of their preference for the generator, either using fine-tuning or prompting.

3.2 QA Evaluator

Inspired by the evaluation metrics introduced in HoneyBee (Song et al., 2023), we develop a comprehensive evaluation metric, RACAR, which consists of five dimensions: **Relevance**, **Agnosticism**, **Completeness**, **Accuracy**, and **Reasonableness**.

- **Relevance** quantifies *how relevant* generated QA pairs are to the information presented in the source article. The generated questions are required to ask about the facts and knowledge provided in the article.
- Agnosticism: We require that the generated questions must not refer to demonstrative content from the original text, like figures or tables in the provided dataset. This dimension of the metric measures the degree of contextindependence of the generated questions.
- Completeness assesses whether the answer comprehensively covers all relevant aspects of the question and effectively utilizes the details in the paper.
- Accuracy measures how well the generated answer corresponds to the relevant facts or information presented in the given paper. Any claims or statements in the answer should be supported by evidence from the paper.
- Reasonableness pertains to the internal logic within the generated answer. It involves assessing whether the answer is logically coherent without contradictions.

To measure alignment between GPT-4 and human evaluation, we engaged two domain experts to manually evaluate the 10 QA pairs for 10 articles

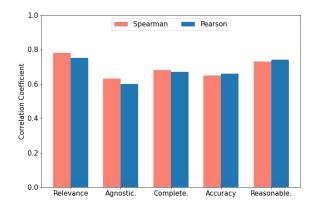


Figure 2: Spearman and Pearson correlations between GPT-4 assigned scores and expert-annotated scores.

(a total of 100 pairs) with the same RACAR metric. Figure 2 shows the averaged spearman and pearson correlations between GPT-4 assigned scores and expert-annoted scores.

Our evaluator serves two purposes: 1) evaluating the quality of the generated QA pairs, and 2) acting as a filter to discard low-quality QA pairs after establishing a standard. It is noteworthy that this standard is customizable; it can be a score threshold or a selection of the top k QA pairs based on their overall ranking. In this study, we directly use GPT-4 as QA evaluator to evaluate the generated QA pairs (see Appendix C for prompts) along these dimensions on a scale of 1–5, with 1 being unacceptable and 5 fully acceptable. Users of this framework can select any open-source or cosed-source LLM for evaluator, either using fine-tuning or prompting.

4 SciQAG-24D Dataset

4.1 Paper collection

From the Web of Science (WoS) Core Collection database, we obtained scientific papers that met the following criteria: 1) categorized in physical science disciplines (materials science, chemistry, physics, energy); 2) available in full-text HTML/XML format from publishers like Elsevier, Springer Nature, and Royal Society of Chemistry; and 3) written in the English language (see Appendix A for details). We selected 24 WoS categories and for each WoS category, we selected most highly cited papers and employed the Sci-Crawler paper downloading tool (Xie et al., 2023a) to retrieve their content in plain text format. This dataset of 22,743 papers aims to serve as a cred-

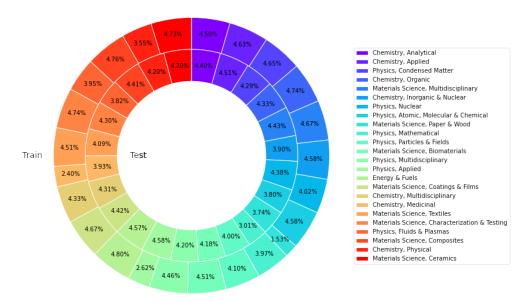


Figure 3: Proportion of papers of different categories in the training and testing of the SciQAG-24D dataset.

ible, rich, balanced, and representative source of scientific knowledge. The number of papers selected for each category can be found in Table 4 in Appendix B.

4.2 Using the SciQAG Framework

To fine-tune an open-source LLM as QA generator, we first randomly selected 426 papers from the paper collection as input to produce 4260 seed QA pairs by prompting GPT-4 (see Appendix C). Then, we fine-tuned vicuna-7b-v1.5-16k model (Zheng et al., 2023) on seed data. The data employs the instruction schema (Wang et al., 2022) composed of three elements: <instruction>, <input>, and <output>. The seed QA generation prompt was converted into the <instruction>. The seed paper filled the <input> field, and the <output> were the generated seed QA pairs. We concatenated the instruction and instance input as a prompt and train the model to generate the instance output in a standard supervised way. It is instructive to compare the SciQAG science QA generator with the self-questioning prompting approach of Fang et al. (2024), which as we show in Appendix F can also be used to generate factual QA pairs from text.

Using the trained QA generator, we performed inference on the remaining papers, generating a total of 227,430 QA pairs (including seed QA pairs). We sampled 50 papers from each category (a total of 1,200 papers) and their generated QA pairs, using GPT-4 to compute the RACAR score for each QA pair. QA pairs with any score lower than 3

were filtered out to form a test set. For the remaining QA pairs, a simple rule-based approach was used to remove all pairs containing "this paper" or "this study" to form a training set.

4.3 Statistics of SciQAG-24D

Overview. Using SciQAG framework, we established our open-ended science QA benchmark dataset, SciQAG-24D, which covers 24 scientific domains. Figure 3 shows the proportion of papers of different categories in the training and testing. And Table 4 in Appendix B lists the categories, the train-test split, the number of papers and generated QAs. The dataset consists of a total of 22,743 original papers, with 21,543 papers used for training set and 1,200 papers for test set. After filtering, the training set includes 21,529 papers and 179,511 QA pairs, while the filtered test set contains 1,199 papers and 8,531 QA pairs. This extensive collection of QA pairs aims to support the development and evaluation of open-ended QA systems in various scientific fields. This dataset has multiple applications: the training set can be used to fine-tune LLMs, infusing them with scientific knowledge; while the test set can be used to evaluate the overall performance of LLMs on open-ended, closedbook science QA tasks, or within specific domains. Given its substantial size, the test set can also serve as high-quality data for fine-tuning. Next, we provide several statistical metrics and visualizations to assess the quality of QA pairs from various perspectives.

Source validation of numeric values. We encourage the generator to reference data from the source paper when generating answers. However, we are concerned about inevitable hallucination (Xu et al., 2024), wherein the model fabricates numbers as support. Given our requirement that both questions and answers stay within the scope of the source paper, we assume that a numerical value in a generated answer that does not occur in the original text has uncertain authenticity. Thus we define the following ratio, which ideally should have value 1:

(1)

We find that 27.29% of generated answers contain numerical information. Of the numeric values found in answers, 99.15% occur in the source text, suggesting that fabricated numerical data are rare.

Diversity of questions: Since we aim for unique questions that are not mere paraphrases of each other, we calculated the text similarity between generated questions. Traditional metrics like ME-TEOR (Banerjee and Lavie, 2005b) fail to capture the true intent behind textually similar questions, as seen in the example:

- What are the advantages of using zeolites?
- What are the disadvantages of using zeolites?

To address this, we use chain-of-thought (CoT) (Wei et al., 2022) prompting with the Mixtral 8×7B model (Jiang et al., 2024) in a few-shot setting (see Appendix E). It instructs the model to predict similarity scores by: 1) understanding the purpose; 2) identifying aspects; 3) comparing intent; and 4) assigning a score. We computed pairwise similarities for sets of 10 questions generated for each of 50 papers. Most questions exhibit dissimilarity (see Figure 4). The distribution of the 2250 similarity scores, calculated from the 50×10×9/2 possible question pairs, reveals that 87.29% of the scores fall below 0.3, while only 2.27% exceed 0.7. The average similarity score of 0.186 demonstrates the effectiveness of the SciQAG method in generating a diverse set of questions with minimal overlap, ensuring that the generated questions are distinct from one another.

Coverage rate of answers. To show our answers are from different parts of the paper, we measure the coverage rate of a paper's associated set of answers A. We first calculate the cosine similarity

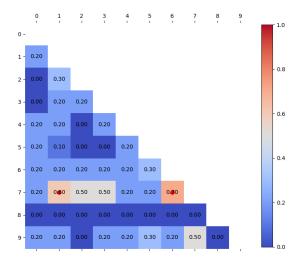


Figure 4: Pairwise similarities between pairs of 10 questions generated from Ivleva et al. (2009). Lower similarity is indicated by bluer cells, while higher similarity is indicated by redder cells. Scores above 0.7 are marked with red dots.

of each answer $a \in A$ to each sentence s in the paper and then construct as S_{15} the set of sentences in the paper that are in the topk (k = 15%) similarity scores for any answer in A. We then divide the paper into 10 equally sized chunks and measure how many of these chunks contain any sentence from S_{15} . The coverage rate is defined as:

$$P_{\text{cov_rate}} = \frac{\sum_{i=1}^{10} \bigcup_{x \in topk(a)} \mathbb{1}_x(C_i))}{100}$$
 (2)

where C_i is the set of sentences in chunk i of the paper $(i \in 1, 2, ..., 10)$, A is the set of generated answers, topk(a) is the set of 15% of sentences in the paper that are the most similar to answer a, and $\mathbb{1}_x(A)$ is the indicator function indicating if $x \in A$.

We calculate a similarity score between each answer and every sentence in the paper using contextual embeddings generated by the e5-mistral-7b-instruct model (Wang et al., 2024). The average coverage rate for the 50 papers randomly selected is 78.6%. Details of how sourcing works in practice are visualized in Appendix G.

5 Experiments

5.1 Experimental setup

To investigate performance differences across various language models and the impact of fine-tuning, we designed a comprehensive experimental setup.

Zero-shot setting. We used part of the test set in SciQAG-24D to conduct a zero-shot comparison of five models. Two of them are open-sourced LLMs: LLaMA1 (7B) (Touvron et al., 2023a) and LLaMA2-chat (7B) (Touvron et al., 2023b). And the rest are commercial LLM systems (use API): GPT-3.5 (gpt-3.5-turbo) (Ouyang et al., 2022), GPT-4 (gpt-4-1106-preview) (OpenAI et al., 2023), and Claude3 (claude-3-opus-20240229) (Anthropic, 2024). Each model was prompted with 1000 questions in test, and their outputs were evaluated by CAR metrics (see Section 5.3 for details) to gauge their zero-shot capabilities in answering scientific research questions.

Fine-tuned setting. Next, we examined the impact of fine-tuning. We fine-tuned LLaMA1 using the training set in SciQAG-24D. This fine-tuned model, LLaMA1-QA, was evaluated on an unseen test set in SciQAG-24D, and its performance was compared against the zero-shot performance of the original LLaMA1. Since the primary purpose of the training set is to fine-tune the model to infuse scientific knowledge, we further explored the performance of LLaMA1-QA after fine-tuning on other scientific tasks. The first task was SciQ (Welbl et al., 2017), a scientific MCQ benchmark and we used 10,000 examples as training data and 1,000 examples as test data. We also conducted evaluations on several other scientific tasks (see Table 5 for details), including different types like classification, regression, and transformation.

5.2 Implementation details

For zero-shot experiments, we set repetition penalty of LLaMA1 to 1.2 and max token length of LLaMA2-chat to 1024. Apart from these specific settings, the rest are configured with repetition set to 1 and the max token length set to 512. To fine-tune the LLaMA1 model on QA pairs, we follow the method of Alpaca (Taori et al., 2023), using a batch size of 1 and a maximum sequence length of 512 tokens. The training process is conducted over 2 epochs using the DeepSpeed Stage 3 optimization framework across 8 AMD GPUs. Gradients are accumulated over 2 steps, and the learning rate is set to 2e-5 with no weight decay. The number of warm-up steps is set to 20. For all inference, we set the temperature to 0.8 and the top_p to 0.75.

5.3 Evaluation metrics

For the evaluation of the quality of generated answers in the zero-shot experiment, we adopt a modified version of the RACAR framework. We exclude the criteria of "Relevance" and "Agnosticism", which are specifically designed to assess the alignment of question-answer (QA) pairs with a given paper, and name this modified metric as **CAR** (see Appendix J). For evaluating performance on SciQ dataset, we utilize the accuracy metric to conduct our evaluations. For evaluating performance on other scientific tasks, we use F1-score for classification tasks, Mean Absolute Error (MAE) for regression tasks, and KL divergence (Brown et al., 2019) for transformation tasks.

6 Results and Analysis

6.1 Zero-shot Evaluation

The results of the zero-shot performance on the SciQAG-24D test are summarized in Table 2. Among the models, GPT-4 achieved the highest scores in Completeness (4.9) and Reasonableness (4.9896), while Claude3 obtained the highest Accuracy score (4.95). GPT-3.5 also performed exceptionally well, with scores closely trailing those of GPT-4 and Claude3 across all metrics. Notably, LLaMA1 scores the lowest in all three dimensions. In comparison, the LLaMA2-chat model, although not as high-scoring as the GPT models, demonstrates substantial improvements over the original LLaMA1 in all metrics. These results highlight the superior zero-shot performance of the commercial LLM models in answering science questions. We can also find that the latest open-source models, such as LLaMA2-chat, have made significant advancements and possess science questionanswering capabilities comparable to commercial LLMs.

6.2 Impact of Fine-tuning

We selected LLaMA1, which exhibited the poorest zero-shot performance, for fine-tuning to obtain LLaMA1-QA. Through three experiments, we demonstrated that SciQAG-24D serves as effective fine-tuning data capable of improving downstream scientific task performance.

SciQAG-24D test. As shown in the last line of Table 2, LLaMA1-QA, demonstrated significant performance improvement compared to the original

Model	Completeness	Accuracy	Reasonableness
LLaMA1	2.7813	2.9625	3.2917
LLaMA2-chat	4.7125	4.4708	4.7625
GPT-3.5	4.8708	4.9333	4.9895
GPT-4	4.9	4.9438	4.9896
Claude3	4.7938	4.95	4.9875
LLAMA1-QA	3.1479 (+13.18%)	3.8875 (+31.22%)	4.3896 (+33.35%)

Table 2: Zero-shot performance on SciQAG-24D test. **Bold** denotes best model scores. As a comparison with LLaMA1, we also show results of LLaMA1_QA in the last line.

Type	Dataset	LLaMA1	LLAMA1-QA
M	SciQ	0.895	0.904
	Glass	0.813	0.872
C	Pei	0.9531	0.960
C	Stability	0.809	0.931
	UV	0.596	0.729
	Bandgap	0.435	0.384
R	Steels	463.959	185.316
K	ChEMBL	1.195	1.180
	Diversity	0.307	0.294
	Ср	4.790	4.645
Т	Stability	0.647	0.824
1	ES0L	0.788	0.829

Table 3: Fine-tuning performance of LLaMA1 and LLAMA1-QA on SciQ and scientific tasks (C for classification; R for regression; T for transformation). The details of datasets are available in Table 5.

LLaMA1 (over 13% in Completeness, and over 30% in Accuracy and Reasonableness). This indicates that LLaMA1 has learned the logic of answering science questions from the training data in SciQAG-24D and internalized some scientific knowledge.

SciQ test. In the first line of Table 3, LLaMA1-QA exhibits a slight improvement over LLaMA1 (+1%). However, based on our observations and statistics, fine-tuning on SciQAG-24D has also enhanced the model's instruction-following ability: the SciQ test requires selecting an option as an answer, but occasionally, LLMs may generate format errors that prevent automatic parsing of the predicted option from the output. The probability of unparseable outputs has decreased from 4.1% with LLaMA1 to 1.7% with LLaMA1-QA.

Scientific tasks. In Table 3, LLaMA1-QA exhibits notable improvements over LLaMA1 model in scientific tasks. The most significant improvement is observed in the Steels regression task, where the MAE decreased from 463.96 to 185.32. These find-

ings indicate that incorporating science QA into the training process can enhance the model's ability to learn scientific knowledge, thereby improving its performance on downstream prediction tasks. Surprisingly, compared to machine learning models specifically designed, LLM can achieve comparable results or even surpass them in certain tasks. For example, in the Bandgap task, although LLaMA1-QA does not perform as well as models like MOD-Net (0.3327), it has already surpassed AMMExpress v2020 (0.4161) (Dunn et al., 2020). In the Diversity task, LLaMA1-QA outperforms the deep learning baseline (0.3198) (Jablonka et al., 2024). These findings demonstrates that LLMs hold significant potential for specific scientific tasks.

7 Conclusion

In this work, we present SciQAG, a novel framework for generating QA pairs from scientific literature, and propose RACAR metrics for evaluating and filtering these QA pairs. SciQAG can cost-effectively produce knowledge-based QA data for low-resource scientific domains, addressing a key challenge in developing science QA systems. Using SciQAG, we create an science QA dataset with 188,042 QA pairs. Its training set can finetune LLMs with scientific knowledge, and its test set can evaluate LLM performance on open-ended, closed-book science QA tasks. To assess the impact of the dataset, we compare the zero-shot performance of several LLMs on the test set and finetune LLaMA1 on the training set, resulting in the LLaMA1-QA model. This fine-tuning significantly improves LLaMA1-QA's performance on the test set (unseen QA), the SciQ test (MCQ), and various scientific tasks (real-world experimental problems). Additionally, this study demonstrates the potential of LLMs in scientific tasks, with LLaMA1-QA achieving results comparable to or surpassing machine learning baselines. These findings highlight the utility of the SciQAG-24D dataset in enhancing LLMs' understanding and application of scientific knowledge. We aim to promote future research in this field, advancing science QA systems and providing valuable resources for practitioners.

Limitations

Firstly, although the questions in the dataset do not explicitly depend on the original text, there may still be implicit dependencies, such as authorspecific terminology or names. This can lead to gap between what the LLM learns during training and real knowledge embedded in the QA pairs. Secondly, hallucinations, while relatively infrequent, are still inevitable due to the inherent nature of LLMs. Even a perfect RACAR score does not guarantee that the generated answer is entirely accurate or factual. Thirdly, the RACAR evaluation framework appears to perform better when using commercial models compared to open-source models, and when assessing each dimension individually rather than all five dimensions simultaneously. However, this approach is more resourceintensive. Future work should explore the balance between computational efficiency and performance to develop more sustainable evaluation strategies. Lastly, the current version of the SciQAG-24D dataset covers a limited range of scientific domains. To enhance the dataset's representativeness and utility, it is crucial for the research community to collaborate and contribute to its expansion, incorporating a wider variety of scientific disciplines and question types.

Ethics Statement

Our research does not raise any major ethical concerns.

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A Complete list of 24 WoS categories and original distribution

- 1. Materials Science, Multidisciplinary
- 2. Physics, Multidisciplinary
- 3. Chemistry, Multidisciplinary
- 4. Materials Science, Coatings & Films
- 5. Materials Science, Ceramics
- 6. Materials Science, Characterization & Testing
- 7. Materials Science, Biomaterials
- 8. Materials Science, Composites
- 9. Materials Science, Paper & Wood
- 10. Materials Science, Textiles
- 11. Physics, Applied
- 12. Physics, Atomic, Molecular & Chemical
- 13. Physics, Condensed Matter

- 14. Physics, Fluids & Plasmas
- 15. Physics, Mathematical
- 16. Physics, Nuclear
- 17. Physics, Particles & Fields
- 18. Chemistry, Analytical
- 19. Chemistry, Applied
- 20. Chemistry, Inorganic & Nuclear
- 21. Chemistry, Medicinal
- 22. Chemistry, Organic
- 23. Chemistry, Physical
- 24. Energy & Fuels

Figure 5 shows the original distribution of 24 categories.

B Statistics of SciQAG-24D dataset

Table 4 shows the details of 24 categories in SciQAG-24D dataset.

C Prompts for QA generator

Here is a scientific paper:

{text}

Here is a two-step task for you.

Step 1: Read given scientific paper and extract a list of 15 keywords focusing on the important terms and concepts within the paragraph. Avoid generic or broad words.

Step 2: Generate 10 scientific Q&A pairs as diverse as possible based on facts and knowledge presented in given paper, focusing on keywords you generated. Keep the following requirements in mind: Avoid ask simple or definitional questions. Please assume that there is no corresponding paper to refer to when asking questions, so ensure that the questions and answers are self-contained (do not refer to external sources like figures or tables, or use demonstrative pronouns such as "this"). Incorporate specific data and insights from the paper to create detailed and informative answers. Ensure that the answers are concise, accurate, and directly related to the corresponding questions.

Please present the generated keywords and question-answer pairs in the following format:

Keywords: [keyword 1], [keyword 2], ..., [keyword15]

Q1: [Question 1]

A1: [Answer 1]

Q2: [Question 2]

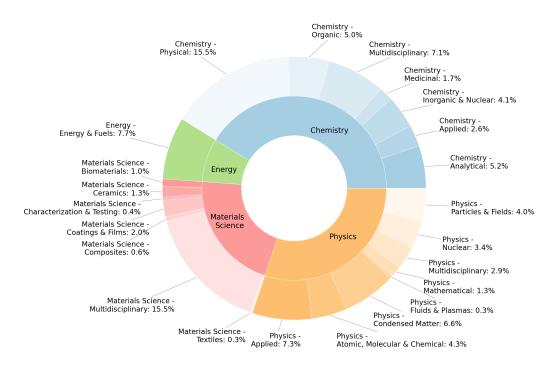


Figure 5: Original distribution of papers from the WoS Core Collection across 24 WoS categories selected from Chemistry, Physics, Materials Science and Energy.

Category	Original	Support (train)				Support (test)	
Category	Paper	Paper	QA	Paper_filter	QA_filter	Paper_filter	QA_filter
Chemistry, Analytical	1020	970	9700	970	8075	50	375
Chemistry, Applied	1037	987	9870	987	8314	50	385
Physics, Condensed Matter	1025	975	9750	974	8340	50	366
Chemistry, Organic	1048	998	9980	998	8513	50	369
Materials Science, Multidisciplinary	1000	950	9500	950	8382	50	378
Chemistry, Inorganic & Nuclear	1024	974	9740	973	8225	50	333
Physics, Nuclear	941	891	8910	888	7208	50	374
Physics, Atomic, Molecular & Chemical	1081	1031	10310	1031	8215	50	324
Materials Science, Paper & Wood	375	325	3250	325	2743	50	319
Physics, Mathematical	1036	986	9860	985	7126	50	257
Physics, Particles & Fields	1000	950	9500	944	7361	50	341
Materials Science, Biomaterials	1007	957	9570	957	8093	50	357
Physics, Multidisciplinary	1000	950	9500	950	8009	50	358
Physics, Applied	581	531	5310	531	4699	50	391
Energy & Fuels	1076	1026	10260	1026	8625	50	390
Materials Science, Coatings & Films	1004	954	9540	954	8390	50	377
Chemistry, Multidisciplinary	952	902	9020	901	7777	50	368
Chemistry, Medicinal	570	520	5200	520	4302	50	335
Materials Science, Textiles	1023	973	9730	973	8095	50	349
Materials Science, Characterization & Testing	1048	998	9980	998	8517	49	367
Physics, Fluids & Plasmas	1016	966	9660	965	7085	50	326
Materials Science, Composites	1046	996	9960	996	8541	50	376
Chemistry, Physical	791	741	7410	741	6380	50	358
Materials Science, Ceramics	1042	992	9920	992	8496	50	358
Sum	22743	21543	215430	21529	179511	1199	8531

Table 4: Statistics of SciQAG-24D dataset.

A2: [Answer 2] A10: [Answer 10]

...

Q10: [Question 10]

D GPT-4 prompts for RACAR metric

Relevance: Given a scientific paper and questions generated from it, evaluate the relevance of the question to the paper and return a score ranging from 1–3 and give reasons as to why this score was assigned. The output must be a list of dictionaries corresponding to each question, with the fields 'score' and 'reasons.' If the question does not pertain to the paper, assign a score of 1.

Paper: { paper_text }

Questions: { [{ questions }] }

Output:

Agnosticism: Given questions generated from a scientific article, evaluate its context independence and return a score ranging from 1–3. Identify whether the question is referring to specific experimental setups, figures, or tables from the paper. For example, questions like "What can we say about the effect of varying pressure from Figure 1?" should be assigned a score of 1. The output must be a list of dictionaries corresponding to each question, with the fields 'score' and 'reasons.'

Questions: { [{ questions }] }

Output:

Completeness: Given a scientific paper and question answer pairs generated from it, evaluate the completeness of the answer for each question and return a score ranging from 1–3 indicating the extent to which the answer fully addresses the question using the information in the paper, including all subquestions. Also give reasons for assigning the score. The output must be a list of dictionaries for each question answer pair, with the fields 'score' and 'reasons.'

Paper: { paper_text }

Questions: { [{ qa_pairs }] }

Output:

Accuracy: Given a scientific paper and question answer pairs generated from this scientific paper, evaluate the accuracy of the answer for each question and return a score ranging from 1–3 indicating whether the answer is accurately extracted from the paper and give reasons as to why this score was assigned. This involves checking the accuracy of any claims or statements made in the text, and verifying that they are supported by evidence.

The output must be a list of dictionaries for each question answer pair, with the fields 'score' and 'reasons.'

Paper: { paper_text }

QA pairs: { [{qa_pairs}] }

Output:

Reasonableness: Given a scientific paper and statements, evaluate the reasonableness of the statements with respect to the paper and return a score ranging from 1–3 indicating how logically consistent the content is, with no obvious contradictions and provide reasons for assigning the score. The output must be a list of dictionaries for each statement, with the fields 'score' and 'reasons.' Assign a score of 1 if the statement has logical error like contradicts.

Paper: { paper_text }

Statements: { [{ answers }] }

Output:

E Prompts for similarity of questions

"""<s> [INST] **Objective**: Assess the similarity of two questions not just based on their word content and relatedness, but primarily based on their underlying purpose or intent. This assessment should distinguish between questions that are about opposite aspects (even if related) and those that are different in wording but similar in the information they seek. Mark it from 0–100. 0 means absolutely no same intention, 100 means completely same intention. You don't need to explain your choice, just output a score in the format of similarity score: <the score>.

- **Procedure**:
- 1. Read and Understand the Questions:
- Carefully read the given questions.
- Understand the core purpose behind each question.
- 2. Identify Key Aspects:
- Determine what each question is specifically asking for.
- Identify if the questions are seeking positive, negative, or neutral aspects of a subject.
- 3. Analyze Semantic Differences:
- Compare the intent behind the questions.
- Look for opposing themes such as benefits vs drawbacks, advantages vs disadvantages, etc.
- 4. Similarity Scoring:

- Assign a high similarity score if both questions are asking about the same aspect of a subject, even if the wording is different.
- Assign a low similarity score if the questions are asking about opposite aspects, even if they are related or use similar words.

Examples:

Question 1: "What are the pros of using zeolites?" Question 2: "What are the drawbacks of using zeolites?"

Analysis: Although both questions are about zeolites, they asks different aspects: positive vs. negative.

Similarity Score: 0

Question 1: "Give some examples of using zeolites as catalysts."

Question 2: "What are potential applications of using zeolites as catalysts?"

Analysis: Both questions seek information on how zeolites are used as catalysts, with slightly different wording.

Similarity Score: 100

Notes:

Pay attention to nuanced language that may indicate different intentions even in closely related topics.

Remember, a high degree of relatedness does not necessarily imply a high degree of similarity in intent.

Ouestions

Question2: sent2 [/INST]"""

Question1: sent1

Self-questioning vs. SciQAG

Self-questioning (Fang et al., 2024)

Prompt:

Given a paragraph of paper, can you ask five questions and give answers that can be directed to the paragraph? List in the format of Question-Answer pair.

Paragraph: {paragraph}

Example GPT-3.5 completion:

Q1: What is being discussed in this paragraph?

A1: This paragraph is discussing the synthesis of one-dimensional carbon nanorods through a self-templated, catalyst-free strategy and the potential application of these nanorods and graphene nanoribbons in supercapacitor electrodes.

Q2: What transforms the nanorods into graphene nanoribbons?

A2: Sonochemical treatment followed by chemical activation transforms the nanorods into graphene nanoribbons.

Q3: What properties of nanomaterials makes them attractive?

A3: The extraordinary electrical, mechanical and thermal properties of one- and two-dimensional carbon nanomaterials makes them attractive.

Q4: What is the major challenge associated with the synthesis of these materials?

The major challenge in the synthesis of these materials is to develop simple and efficient methods that consume low amounts of energy.

What advantages does this particular O5: synthetic approach offer?

A5: This particular synthetic approach offers advantages such as scalability and the production of functionally useful materials on industrial levels.

SciQAG (this paper)

Prompt:

Here is a scientific paper:

{text}

Given the provided scientific paper, please complete the following two steps:

Step 1: Keyword Extraction

Read the scientific paper and identify 15 keywords that capture the most important terms and concepts in the paper, avoiding generic or broad terms. Compile the selected keywords into a list.

Step 2: Question-Answer Generation

Generate 10 science question-answer pairs as diverse as possible based on facts and knowledge presented in the given paper, focusing on keywords you generated. Keep the following requirements in mind: Avoid asking simple or definitional Assume that the reader does not questions. have access to the original paper or any external sources, so ensure that the questions and answers are self-contained and do not rely on references to figures, tables, or other parts of the paper. Incorporate specific data and insights from the paper to provide detailed and informative answers. Keep the answers concise, accurate, and directly related to the corresponding questions.

Please present the generated keywords and question-answer pairs in the following format: Keywords: [keyword 1], [keyword 2], ..., [keyword15]

Q1: [Question 1] A1: [Answer 1]

Q2: [Question 2] A2: [Answer 2]

•••

Q10: [Question 10] A10: [Answer 10]

Example SciQAG completion:

Q1: What is Type 1 diabetes and what causes it? A1: Type 1 diabetes is an autoimmune disease that results from the selective destruction of insulin-producing beta cells in the pancreatic islets. Genetics, environmental factors, nutritional effects, and a combination of these are believed to be associated with the disease. Streptozotocin (STZ) is commonly used to induce diabetes mellitus in experimental studies.

Q2: What is the role of metabolomics in healthcare?

A2: Metabolomics is a rapidly growing field that relates biological end points to multiple altered metabolite concentrations, providing a wealth of biological information on complex systems. It has been applied to a variety of diseases such as cancer, type 2 diabetes, and inborn errors of metabolism. It uses advanced analytical techniques such as nuclear magnetic resonance (NMR) spectroscopy and mass spectrometry with multivariate statistical analysis to identify potential biomarkers and biological networks.

Q3: How was the diabetic rat model established in this study?

A3: In this study, female rats were divided into a diabetic group and a control group. The diabetic group received an intraperitoneal dose of STZ, and showed glucose levels in the blood of more than 200 mg/dl after 4 days. The control group was matched for age and gender, and did not receive the STZ injection.

Q4: What were the key findings regarding glucose metabolism in the study?

A4: The study found that in diabetes, glucose excretion was enormous, being nearly 7500-fold higher than in control rats. Other significantly enhanced metabolites included lactate, alanine, ethanol, and fumarate. These findings suggest that glucose metabolism is dramatically perturbed in diabetes.

Q5: What is the importance of the Cori cycle in maintaining glucose homeostasis?

A5: The Cori cycle, also known as the glucoselactate cycle, is a metabolic pathway that plays a crucial role in maintaining glucose homeostasis. It involves the conversion of glucose, lactate, and alanine, and is responsible for producing Cori cycle intermediates, which are used in gluconeogenesis precursor production and facilitating glucose oxidation.

Q6: What is the role of acetate switch in metabolism?

A6: The acetate switch, also known as the molecular switch that regulates the dissimilation and assimilation of acetate, plays a role in accumulating an acetyl-coenzyme A (CoA) pool due to both exogenous (bacterial fermentation) and endogenous (mammalian) production. This accumulation can have significant implications for metabolism.

Q7: How did the urinary metabolites differ between diabetic and control rats in the study?

A7: The urinary metabolites showed dramatic changes in the rat diabetic model when compared with blood-based assays. Glucose was the most notable metabolite in diabetic urine, with very high-intensity signals. Other metabolites such as alanine, lactate, ethanol, acetate, and fumarate also showed significant increases in the diabetic group.

Q8: What was the effect of STZ administration on plasma glucose levels?

A8: Following STZ administration, plasma glucose showed elevated levels, with its quantity being nearly three times higher than in control rats.

Q9: What were some of the changes observed in the rat diabetic model's blood parameters?

A9: Other than the significant increases in blood glucose levels, the study also observed elevated levels of urea and creatinine, and decreased levels of plasma protein and cholesterol in diabetic rats.

Q10: How did the correlations among the detected metabolites differ between the diabetic and control rats?

A10: The correlations among the detected metabolites showed a number of striking differences between the diabetic and control rats. For example, the correlation of glucose with alanine was increased in diabetic rats, while the correlation of glucose with lactate decreased. These changes indicate significant alterations in metabolism in the diabetic rats.

Analysis:

Due to the nature of its prompting technique, self-questioning is prone to generate more generic and contextually tied questions (e.g., "What is being discussed in this paragraph?"). SciQAG is able to avoid self-referential expressions such as 'this,' 'that,' and 'these,' making it more suitable for crafting challenging closed-book QA datasets, though this may slightly compromise its compatibility with source papers for open-book QA applications.

The scope of questions generated by SciQAG is notably broad and deep. Unlike simpler, definitionfocused queries, SciQAG explores various aspects such as relevant properties, application impacts, strategic influences, structural differences, challenges, and experimental insights. This diversity ensures that the questions not only span a wide range of topics but also deeply engage with the subject matter of the scientific papers. The answers produced by SciQAG are equally impressive in their informativeness and specificity. They meticulously avoid over-generalization, often incorporating precise details like specific chemical elements and numerical values that are referenced in the original papers. This level of detail in the answers highlights the method's ability to maintain relevance and accuracy in relation to the scientific content. The comparison between SciQAG and selfquestioning thus underscores SciQAG's strengths in generating diverse, context-independent, and content-rich QA pairs.

G 10 generated questions example

The following 10 questions were generated from a random paper Ivleva et al. (2009) by QA generator.

Q1: What are the applications of rapid diagnostic assays as discussed in the paper?

Q2: What is the significance of mycotoxin detection in the food and feed sector?

Q3: What are the advantages of lateral-flow devices (LFDs) in the context of rapid immunoassay-based tests?

Q4: What are the potential applications of LFDs according to the paper?

Q5: What are the challenges in the development of rapid test strips for mycotoxins?

Q6: What is the significance of antibody sensitivity and specificity in the performance of a membrane-based immunoassay?

Q7: What extraction procedures are commonly used for mycotoxin analysis?

Q8: How does matrix variation affect the results of rapid tests for mycotoxins?

Q9: What is the role of colloidal gold in test strips for mycotoxins?

Q10: How do regulatory limits vary for mycotoxins in different countries?

H Pairwise visualization

We show in Figure 6 (a) and (b) the top 10 sentences with the highest similarity scores for each answer generated for two articles selected at random from our collection. We observe that some sentences serve as common sources for multiple answers; however, overall, there tend to be distinct sources for each answer. Additionally, we plot

heatmaps to provide a holistic view of the similarity scores between each answer and all sentences in the paper. Figure 6 (c) and (d) offer a thorough overview of the connections between answers and various parts of the given paper (a & c, b & d are from the same paper). From the perspective both of coverage and sourcing rates, and of the two visualization methods, it is evident that the answers generated by SciQAG exhibit extensive coverage of the source paper and originate from diverse sources.

I Details of generating SciQAG-24D dataset

We employ the gpt-4-1106-preview model with its default parameter settings for the seed QA generation and RACAR evaluation. We follow the training method from LongLoRA (Chen et al., 2023) and fine-tune the vicuna-7b-v1.5-16k model (Zheng et al., 2023) using Flash-Attention2 (Dao, 2023) and DeepSpeed (Rasley et al., 2020) stage 3 on an 8×A800 GPU machine for 5 epochs with a per-device batch size of 1 and max length of 16,000 for both training and evaluation. Gradients were accumulated over 2 steps and the learning rate was set to 2e-5 with no weight decay. The warm-up steps were set to 20. For inference, we set temperature to 0.8 and top_p to 0.75, which makes text generated more logical with rich vocabulary.

J Prompts for CAR metric

For this task, you are provided with a questionanswer pair. Evaluate the quality of answer on the following three criteria and record your evaluations in a score ranging from 1 to 5 for each criterion and provide reasons for assigning the score:

- 1. **Accuracy**: Score the accuracy of the answer in relation to the question. A score of 5 means the answer is fully accurate. This involves checking the accuracy of any claims or statements made in the text, and verifying that they are supported by evidence. While a score of 1 indicates significant inaccuracies.
- 2. **Completeness**: Rate how comprehensive the answer is. A score of 5 indicates that the answer addresses all key points of the question and includes sufficient background and supporting details and evidence. A score of 1 means the answer is largely incomplete.
- 3. **Reasonableness**: Evaluate the logical

consistency and reasonableness of the answer. A score of 5 indicates that the answer is logically sound with no contradictions; a score of 1 indicates that the answer contains major contradictions.

Provide the scores in a dictionary output. The dictionary is with three keys (name of 3 criterions). The value is a tuple (score and comment).

```
**Example JSON Output:**

"'json
{{"Accuracy": (score, "reason"), "Completeness": (score, "reason"), "Reasonableness": (score, "reason")}}

"*Input Sections:**
- **Question & Answer Pair**:
{qa}

**Output:**
```

K Summary of datasets in scientific tasks

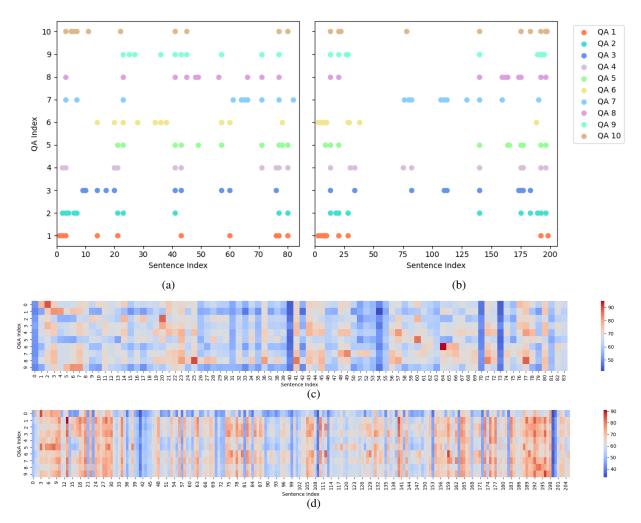


Figure 6: Pairwise similarity from Krska and Molinelli (2009) and Ivleva et al. (2009), respectively. (a) and (b): The 10 sentences with the highest similarity scores. (c) and (d): Heatmap of all similarity scores.

Datasets	Description	Task	
Glass (Kawazoe et al., 1997)	This dataset is retrieved from a volume of the Lan-		
	dolt- Börnstein collection 'Nonequilibrium phase		
	diagrams of ternary amorphous alloys', containing		
	data on full bulk metallic glass formation ability for		
	5680 chemical formulas.		
Pei (Pei et al., 2020)	The dataset is from a thermoelectric material review	С	
	paper published in 2013, which abstracts information		
	from over 100 publications. We used data of 1028		
	materials from this database.		
Stability (Batra et al., 2020)	Consists of water stabilities for over 200 MOFs	C & T	
	(metal-organic frameworks), alongside a comprehen-		
	sive set of chemical features encompassing the metal		
	node, organic ligand, and metal-ligand molar ratios.		
UV (Beard et al., 2019)	Auto-generated UV/vis absorption spectra records	С	
	from 402,034 papers with 18,309 records. We used		
	SMILES to predict category of absorption region		
	(4126 training samples and 1032 test samples).		
Bandgap (Zhuo et al., 2018)	This dataset is retrieved from Zhuo et al.'s work,	R	
	containing data on experimental band gaps and DFT		
	calculated zero band gaps for 4604 compounds.		
Steels (Dunn et al., 2020)	This dataset is retrieved from Citrine informatics,	R	
	containing data on steel yield strengths from compo-		
	sition for 312 chemical formulas.		
ChEMBL (Gaulton et al., 2012)	This dataset is sourced from a curated database of	R	
	bioactive molecules with drug-like properties, focus-		
	ing on the lipophilicity of 1899 molecular compounds		
	in pharmacokinetics. The water-octanol partition co-		
	efficient (logD) is used to describe lipophilicity.		
Diversity (Moosavi et al., 2020)	A diverse set of structures based on the chemical and	R	
	geometric descriptors.		
Cp (Moosavi et al., 2020)	Dataset for predicting the heat capacity of materials	R	
	based on density functional theory simulations.		
ESOL (Delaney, 2004)	This dataset is a compilation of measured aqueous	T	
	solubility (LogS) values, a crucial factor in drug dis-		
	covery. The dataset comprises 927 molecular com-		
	pounds originally used for ESOL - estimated solubil-		
	ity.		

Table 5: Details of datasets and associated tasks they are used to derive instructions, (C for classification; R for regression; T for transformation)