Knowledge Graph Question Answering for Materials Science (KGQA4MAT): Developing Natural Language Interface for Metal-Organic Frameworks Knowledge Graph (MOF-KG)

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Abstract

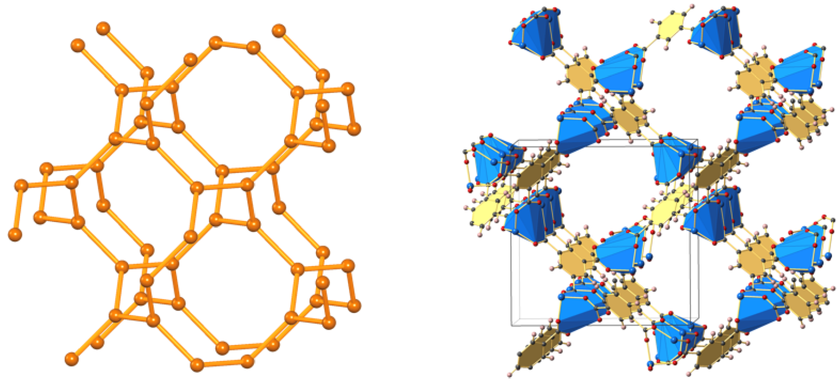
We present a comprehensive benchmark dataset for Knowledge Graph Question Answering in Materials Science (KGQA4MAT), with a focus on metal-organic frameworks (MOFs). A knowledge graph for metal-organic frameworks (MOF-KG) has been constructed by integrating structured databases and knowledge extracted from the literature. To enhance MOF-KG accessibility for domain experts, we aim to develop a natural language interface for querying the knowledge graph. We have developed a benchmark comprised of 161 complex questions involving comparison, aggregation, and complicated graph structures. Each question is rephrased in three additional variations, resulting in 644 questions and 161 KG queries. To evaluate the benchmark, we have developed a systematic approach for utilizing ChatGPT to translate natural language questions into formal KG queries. We also apply the approach to the well-known QALD-9 dataset, demonstrating ChatGPT's potential in addressing KGQA issues for different platforms and query languages. The benchmark and the proposed approach aim to stimulate further research and development of user-friendly and efficient interfaces for querying domain-specific materials science knowledge graphs, thereby accelerating the discovery of novel materials.

Keywords knowledge graph question answering · metal-organic frameworks · pre-trained large language models · natural language interface

1 Introduction

Metal-organic frameworks (MOFs) are a class of porous materials with high surface area, high porosity, and tunable pore size [1], which make them attractive for a wide range of applications, including gas storage, separation, catalysis, and drug delivery. Despite their potential, Metal-Organic Frameworks (MOFs) have yet to be fully utilized due to a lack of comprehensive and systematic knowledge about their composition, structure, synthesis, and properties.

A MOF consists of metal ions or clusters connected by organic ligands, forming a three-dimensional network. Figure 1 illustrates the porous structure and underlying net of the 'MOF-3' that has been extensively studied for various applications in the literature [2]. The ability to tune MOF properties through composition variations results in a very large number of potential MOF candidates. There has been a significant push to use computational techniques to identify the best MOF structures for various applications. As a result, several extensive databases of both synthesized and theoretical MOF structures [3, 4, 5] have been created. In the Cambridge Structural Database (CSD) [3], a leading database that compiles and maintains crystal structures of small-molecule organic and metal-organic compounds, there are more than 100,000 MOF structures that have been documented as of 2022. Additionally, more than 500,000 MOFs have been predicted and stored in other databases [5, 4]. Because it is infeasible to synthesize and test all MOF candidates, identifying optimal MOFs for a target application is a extremely challenging task, akin to trying to find a needle in a haystack.



(a) Underlying net srs

(b) Framework MOF-3 $Zn_2(NO_3)(BTC)$ ($P2_13$)

Figure 1: The Underlying Net and Framework of MOF-3

The MOF identification problem is further compounded by the fact that much of the vital information on MOF synthesis is not found in MOF databases, but scattered throughout scientific literature. Manually searching through thousands of articles to analyze synthesis conditions for a specific MOF structure is both time-consuming and ineffective. To address the problem, several lines of research have applied Natural language processing (NLP) to extract synthesis information from the literature [6, 7, 8]. However, these studies do not create a comprehensive knowledge graph encompassing all aspects of MOFs.

To fully utilize the scattered information generated by MOFs research and experiments, it is essential to gather and integrate the structural information from MOF databases as well as the synthesis procedures in the literature in a easily accessible and searchable place. To this end, we integrated the MOF structural information in several MOF databases with the synthesis procedures extracted from the literature by a recent study [8], resulting in a comprehensive knowledge graph for metal-organic frameworks called MOF-KG [9, 10, 11].

A knowledge graph can be stored in an RDF triple store or in the Neo4j platform. Unfortunately, for either type of system, there is a significant technical barrier for domain experts to directly utilize the knowledge graph. In particular, it is challenging for domain experts to write SPARQL or Cypher queries. To enhance the usability and accessibility of the MOF-KG for domain experts, we aim to develop an intuitive interface that can translate domain experts questions in natural language to corresponding SPARQL or Cypher queries.

In this paper, we introduce a benchmark dataset for Knowledge Graph Question Answering for Materials Science (KGQA4MAT). The benchmark contains 161 complex natural language questions including comparison, aggregation, and complicated graph structures. For each question, we generate three different variations, resulting in total 644 questions. Each question is associated with a corresponding formal query on the underlying graph system. For the current version of the KGQA4MAT benchmark, we focus on Cypher queries on the Neo4j platform.

To evaluate the benchmark, we have developed a systematic approach of utilizing ChatGPT for translating natural language questions into formal KG queries. We also apply the approach to the well-known QALD-9 dataset [12] demonstrating ChatGPT's potential addressing KGQA issues for different platforms and query languages. The benchmark, MOF-KG, and the proposed approach aim to stimulate further research and development of user-friendly and efficient interfaces for querying domain-specific materials science knowledge graphs, thereby accelerating the discovery of novel materials.

The rest of the paper presents the MOF-KG, the KGQA4MAT benchmark, the proposed approach, and evaluation results for question answering over the MOF-KG. Section 2 presents related work. Section 3 describes the MOF-KG. Section 4 discusses the challenges of translating NL questions against the MOF-KG. Section 5 presents the KGQA4MAT benchmark. Section 6 describes the proposed approach for KGQA. Section 7 describes the evaluation results. Section 8 discusses the findings. Finally, Section 9 concludes the paper and presents future directions.

2 Related Work

Researchers have begun to develop knowledge graphs in different materials areas [13, 14, 15, 16]. MMKG [13] is a knowledge graph derived from DBpedia and Wikepedia for Metallic Materials. Propnet [14] is a Python framework to create a knowledge graph by connecting materials in existing datasets through their properties. NanoMine [15] is a curated knowledge graph (KG) that has been developed for the field of nanocomposite materials science. MatKG [16] is a large KG that contains general materials science concept and relationships extracted from 4 million materials science-related papers. Despite the potential benefits of KGs for materials research, there is a lack of KGs specifically tailored to the field of metal-organic frameworks (MOFs).

KGs must be easily searchable by domain experts using simple and intuitive methods. Most existing materials science KGs were inadequate in this aspect as they require the end users to use a highly specialized query languages. Knowledge Graph Question Answering (KGQA) aims to enable end users to pose natural language questions and receive answers from knowledge graphs (KGs) [17]. Benchmark datasets are crucial for evaluating the performance of KGQA systems and fostering advancements in the field. The creation of such datasets usually involves the development of a set of complex questions with varying degrees of difficulty, covering diverse topics and targeting different KG representations. Some well-known benchmark datasets include QALD series [12], LC-QuAD series [18, 19], and SciQA [20]. Steinmetz et al. in [21] surveyed the challenges associated with the creation of many existing KGQA benchmarks.

While the benchmarks such as QALD, LC-QuAD, and SciQA have become influential for assessing and advancing the state-of-the art in KGQA, they mainly target at general knowledge based on large open general knowledge graphs such as DBpedia, Wikipedia, and ORKG. There lacks benchmarks on specific domain knowledge graphs such as in materials science. As KGQA systems continue to evolve, the development of more comprehensive and diverse benchmark datasets will remain essential for future progress.

Several KGQA systems have been developed over the years, each with distinct techniques for translating natural language questions into formal SPARQL or Cypher queries. Early systems employed rule-based or template-based approaches [22]. Recent KGQA systems have increasingly adopted machine learning and deep learning techniques. Techniques such as sequence-to-sequence models, attention mechanisms, neural machine translation, and graph neural networks [23, 24, 25, 26, 27] have been employed. Despite the significant progress in the field, several challenges remain to be addressed, such as handling complex queries with multiple relations, aggregations, or comparisons. Since the emergence of pre-trained Large Language Models (LLM) and ChatGPT, a flurry of studies have been proposed on extracting knowledge graphs [11, 28] and evaluating ChatGPT for KGQA [29, 30, 31, 32]. The KGQA Github repository[1] contains rich KGQA resources including datasets, systems, and leaderboard. The most recent leaderboard indicates that KGQA remains a challenging problem demanding continued research to develop more accurate and robust systems.

3 The MOF Knowledge Graph (MOF-KG)

The MOF Knowledge Graph (MOF-KG) is a comprehensive representation of knowledge related to metal-organic frameworks, encompassing various aspects such as structures, properties, and synthesis procedures. To build the knowledge graph, we began with defining an ontology and then populated the knowledge graph with the data in MOF databases such as Cambridge Structural Database (CSD) [3] and the extracted synthesis procedures from the literature.

Currently, a universally accepted system for describing metal-organic frameworks (MOFs) and related phenomena remains nonexistent. Although a few initiatives have been established to standardize the nomenclature [33, 34], their

[1] https://github.com/KGQA/leaderboard

scope and applicability in integrating MOF information into a comprehensive knowledge graph are limited. Several domain-specific materials science ontologies exist, such as Ashino's Materials Ontology [35], ChEBI (Chemical Entities of Biological Interest) [36], Elementary Multiperspective Material Ontology (EMMO) [37], Materials Design Ontology (MDO) [38], and the NIST controlled vocabulary [39]. Additionally, the MatPortal project [40] serves as an open repository, a massing over 20 ontologies related to materials science. However, none of these ontologies specifically address the distinct concepts and relationships inherent to MOFs.

In our previous work [10], an ontology for the Metal-Organic Framework Knowledge Graph (MOF-KG) was established, consisting of four primary domains: *synthesis*, *structure*, *atomic composition*, and *publication*. This ontology was refined through the integration of knowledge from structured MOF databases and the extraction of information from relevant literature. Figure 2 illustrates the concepts and relationships within the ontology.

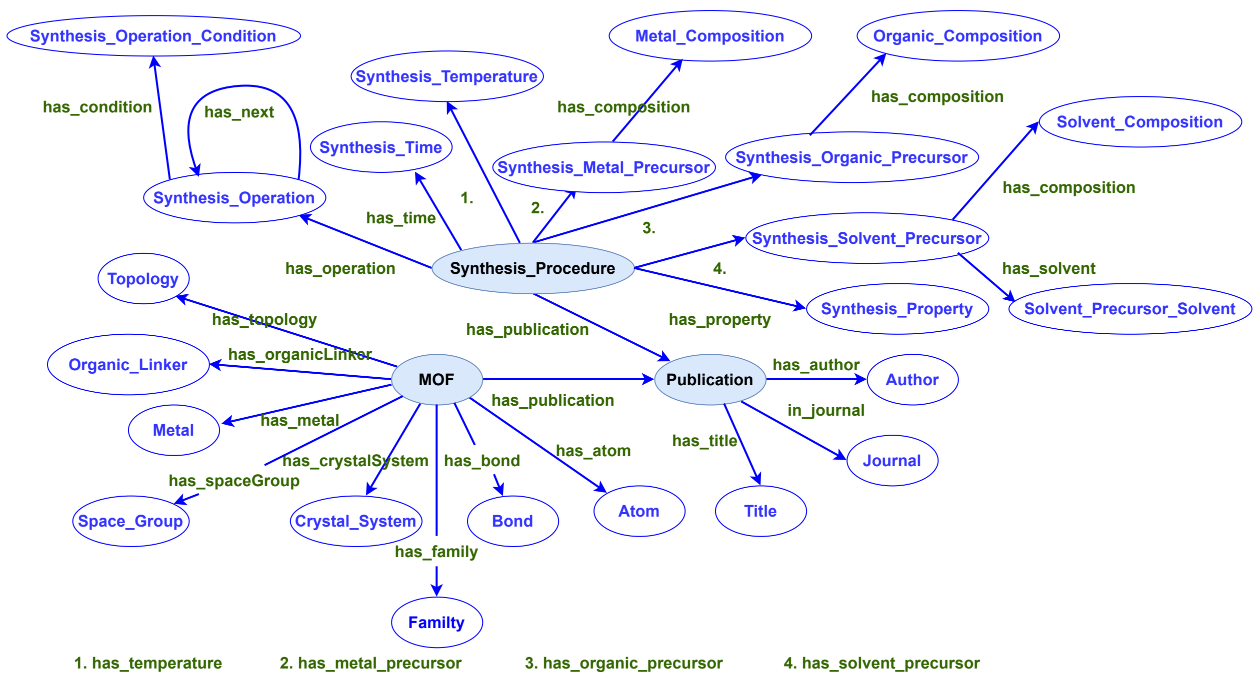


Figure 2: The concepts and relationships in the ontology for the MOF knowledge graph (MOF-KG)

Three key concepts form the foundation of the ontology: MOF, Publication, and Synthesis_Procedure. The MOF concept connects to the concepts representing MOF structure and atomic composition, while the Synthesis_Procedure concept relates to the concepts describing synthesis operations, precursors, and various properties. The Publication concept links to the concepts regarding authors, journals, and titles. Notably, the Publication serves as a cut vertex in the ontology graph, connecting MOF entities to their corresponding synthesis procedures.

The ontology reflects the absence of naming conventions for MOFs and the organization of the information in the original sources. In particular, a database such as the Cambridge Structural Database (CSD) assigns a unique reference code, RefCode, to a MOF, which is associated with a scholarly publication that describes synthesis procedures in the main text or supplemental materials. However, when a publication initially presents the synthesis procedures for one or multiple MOFs, there are no assigned RefCodes yet. Moreover, the naming of MOFs lacks a commonly accepted format, making MOF names unsuitable for identification. Therefore, the MOF knowledge graph (MOF-KG) utilizes the publication's globally unique DOI to bridge the MOFs and the synthesis procedures, thus creating a cut vertex.

The MOF knowledge graph (MOF-KG) is populated by the information extracted from the MOF collection[2] in the CSD database, the CoRE MOF dataset[3] created by Chung et al. in [41], the MOFs in the Reticular Chemistry Naming and Numbering (RCNN) Database[4], and the synthesis procedures[5] extracted by Park et al. in the study [8]. The following steps describe how to create the MOF-KG from the sources with an appropriate CSD license:

[2]https://www.ccdc.cam.ac.uk/free-products/csd-mof-collection/
[3]https://zenodo.org/record/3370144#.ZDvtN3bMIdV
[4]https://globalscience.berkeley.edu/database
[5]https://doi.org/10.6084/m9.figshare.16902652.v3

1. Download the MOF collection, CoRE dataset, RCNN dataset, and the extracted MOF synthesis procedures.
2. Query the CSD crystal database using licensed CSD Python API to extract the information about crystal system and space group
3. Apply the CSD ConQuest tool to identify a MOF's family by applying the search criteria developed by Moghadam et al. in [42]. There are six prototypical MOF families identified: Zr-oxide nodes (e.g. UiO-66), Cu–Cu paddlewheels (e.g. HKUST-1), ZIF-like, Znoxide nodes, IRMOF-like, and MOF-74/CPO-27-like materials.
4. Leverage the MOFid system[6] developed by Bucior et al. in [43] to identify a MOF's metals, organic linkers, and topology.
5. Populate the MOF-KG by directly mapping the extracted data to the ontology in Figure 2.

The resulting knowledge graph consists of more than 1.5 million nodes and more than 3.7 million relationships between the nodes. The knowledge graph is stored in the Neo4j platform, partially due to its intuitive graph representation and visualization capabilities.

4 Knowledge Graph Query Answering (KGQA) over the MOF-KG

Despite the user-friendly graphical user interface provided by the Neo4j platform, domain experts still face challenges in querying the knowledge graph. One challenge is the need to learn a formal query language, such as Cypher. Another challenge involves understanding the underlying graph structure and schema. Additionally, formulating complex queries to address domain-specific questions can be difficult. The problem of Knowledge Graph Question Answering (KGQA) over the MOF-KG involves enabling users to ask natural language questions about MOFs. There are multiple obstacles associated with KGQA over the MOF-KG:

- *Diverse Query Types*: MOF-KG contains a wide range of information, such as synthesis procedures, structures, atomic compositions, and related publications. Therefore, a KGQA systems should be able to handle a variety of query types, including single- and multi-relation queries, as well as more complex queries involving aggregation, comparison, and negation.
- *Ambiguity and Paraphrasing*: Natural language questions can be ambiguous, contain synonyms, or be phrased in multiple ways. A KGQA system should be able to understand and disambiguate user questions and recognize different ways of asking the same question.
- *Domain-Specific Language*: MOFs and their associated information are often described using domain-specific jargon, chemical formulas, or notation. A KGQA system should be capable of understanding and handling such domain-specific language to provide accurate answers.

Assessing the performance of a KGQA system over the MOF-KG can be challenging due to the specialized nature of the domain and the lack of comprehensive benchmark datasets. Developing suitable evaluation metrics and datasets is essential for driving advancements in KGQA systems for MOFs, and materials science more broadly. In the subsequent sections, we outline a dedicated effort to establish a benchmark dataset specifically designed for assessing the performance of KGQA systems over the MOF-KG. This effort leverages the exceptional capacity of ChatGPT to incorporate a diverse range of question types, domain-specific language, and complex relationships found within the MOF-KG.

5 Developing a KGQA4MAT Benchmark Dataset over the MOF-KG

We began developing our benchmark dataset by generating questions and corresponding Cypher queries involving facts, comparison, superlative, and aggregation. We created 161 such questions. For each question, we asked ChatGPT to rephrase it in 3 different ways. Finally, we have 644 questions. We split the data into train and test sets by the ratio 80:20. As a result, the train set contains 515 questions and queries and the test set contains 129 questions and queries. In the process of translating a question to a query, a KGQA system should prioritize the logical steps underlying the query and treat MOF identifications as interchangeable variables. Consequently, to ensure that MOF identifications do not play a crucial role in the translation, we substituted the MOF-related identifications in the test set with different ones from the training set.

[6]https://github.com/snurr-group/mofid

Promt: `Explain the reasoning in the Cypher query in logical steps. Use normal words in the explanation. No comments. Output the explanation only.`

Figure 3 illustrates the process of generating the benchmark. First, the concepts and relationships within the MOF-KG ontology are incorporated into the prompt provided to ChatGPT. Example definitions are:
`"MOF":["refcode":ID, "name", "refcode"];`
`"Publication":["doi":ID, "year", "first_page", "volume"];`
`"Synthesis_Procedure":["syn_id":ID, "name", "symbol", "method"];`
`"(:MOF)-[:has_publication]-(:Publication)";`
`"(:Synthesis_Procedure)-[:has_publication]-(:Publication)";`
Next, ChatGPT is instructed to generate complex questions based on the MOF-KG definitions. Subsequently, human experts examine and revise the raw questions produced by ChatGPT to create a set of polished questions. In the fourth step, knowledge graph experts convert the refined questions into corresponding Cypher queries for the MOF-KG. Following this, ChatGPT is prompted once more to rephrase the refined questions in at least three distinct ways. Lastly, the original questions, their variations, and the corresponding Cypher queries collectively constitute the benchmark dataset.

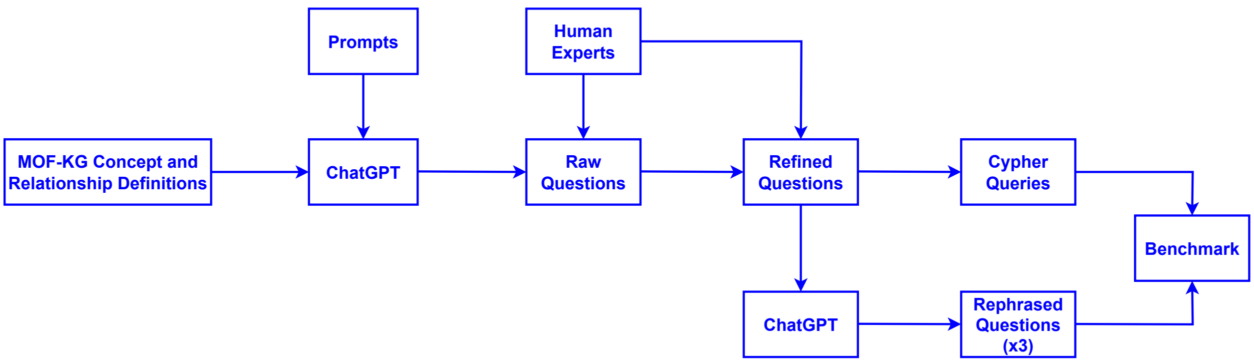


Figure 3: The process of generating the KGQA4MAT benchmark

6 Leveraging ChatGPT to Translate User Questions to KG Queries

ChatGPT, a powerful large language model (LLM), has achieved remarkable progress in the domain of natural language understanding. Owing to its extensive coverage of resources such as Wikipedia and its capacity to support natural language question answering, ChatGPT has attracted attention as a potential alternative to traditional knowledge-based question answering (KBQA) models. However, the utilization of ChatGPT for translating user questions into queries on specific knowledge graphs still requires extensive evaluation.

In order to assess ChatGPT's performance in understanding user questions and generating Cypher queries, we propose an approach that employs zero-shot, few-shot, and chain-of-thought [44] strategies. This approach aims to provide a comprehensive evaluation of ChatGPT's effectiveness in addressing the complexities associated with KGQA and facilitating its application to domain-specific knowledge graphs.

For few-shot learning, the approach needs to find the most semantically similar training questions for a test question. We leverage OpenAI's `text-embedding -ada-002` embedding model to embed all the training and test questions. We then compute the cosine similarity between two embedding vectors for the similarity between the two associated questions. For chain-of-thought [44] reasoning, we first instruct ChatGPT to generate the chain of thought for a given Cypher query, then refine the reasoning steps manually. Our prompt is as follows:

For example, given the Cypher query answering the question: *In what order were the synthetic operations performed to create MOF-3?*, the chain-of-thought explanations are as follows:

After pre-processing the train and test questions and queries, We proposed an approach of leveraging ChatGPT for KGQA with the following methods:

- **Method 0: Answering questions directly.** Ask ChatGPT to answer the users question directly without user-provided additional information.

```
1. Find all MOFs that have a relation "has_publication" to a "Publication".
2. Find all synthesis procedures that have a "has_publication" relation to
   the same "Publication".
3. Find all synthesis operations that are part of the previously found
   synthesis procedures.
4. Filter the MOFs to only include those whose name contains "MOF-3".
5. Output the synthesis procedure id, name of the operation, and the order
   of the operation.
6. Sort the output by the synthesis procedure id in ascending order,
   followed by the operation order in ascending order.
```

- **Method 1: Zero-shot learning from ontology only.** In this method, we prompt ChatGPT with the definitions in an ontology. We then instruct ChatGPT to translate a user question to a Cypher query based on the ontology.
- **Method 2: few-shot learning from a few pairs of train question and query.** Using the embeddings of the test and train questions to find a few highly similar train questions to the test question. Prompt ChatGPT with the pairs of matched train question and query. Instruct ChatGPT to translate the test question to a Cypher query.
- **Method 3: few-shot learning from an ontology and a few pairs of train question and query.** As in Method 2, include an ontology in the prompt, in addition to a few pairs of matched question and query.
- **Method 4: few-shot learning from a few pairs of train question and query, and the chains-of-thought of the train queries.** As in Method 2, include the chains-of-thought of the train queries in the prompt, in addition to the pairs of matched question and query.
- **Method 5: few-shot learning from an ontology and a few pairs of train question and query, and the chains-of-thought of the train queries.** As in Method 3, include the chains-of-thought of the train queries in the prompt, in addition to the definitions in an ontology and the pairs of matched question and query.

7 Evaluation

We evaluate the proposed approach on the KGQA4MAT benchmark. To assess the generalizability of leveraging ChatGPT for KGQA, we also evaluate the approach on the well-known QALD-9 dataset [12]. We apply the OpenAI model `gpt-turbo-3.5` for ChatGPT batch processing. The underlying KG management system of the MOF-KG is Neo4j, while the QALD-9 dataset is over a DBpedia SPARQL endpoint. Thus, our evaluation assesses the performance of ChatGPT on translating user questions to both Cypher and SPARQL queries.

7.1 Evaluation on the KGQA4MAT Benchmark

Since MOF-KG is a domain specific knowledge graph, we evaluate the Method 1-5 in the proposed approach on KGQA4MAT benchmark without asking ChatGPT to answer questions directly. For each translated Cypher query, we execute it on the MOF-KG Neo4j database. We then compare the results to that retrieved by the correct Cypher query to see whether the translated query is correct. We measure the performance using the precision, recall, and F1-score in terms of the correctness of the translated queries:

$$prcision = \frac{\textit{\# of correctly translated queries}}{\textit{\# of total translated queries}} \tag{1}$$

$$recall = \frac{\textit{\# of correctly translated queries}}{\textit{\# of total correct queries}} \tag{2}$$

$$F1\_score = 2(\frac{1}{precision} + \frac{1}{recall})^{-1} \tag{3}$$

For the few-shot methods, we tested using 1, 3, and 5 training examples. We did not see significant differences between the results of using 1, 3, or 5 training examples. We used 1-shot learning to evaluate the full benchmark in order to conserve tokens when utilizing ChatGPT. Table 1 shows the evaluation results.

Because we translated one query for each test question, the total number of translated questions equals to the total number of correct questions. As a result, $precision = reall = F1\_score$. The results demonstrate that our approach

Evaluation Method on the KGQA4MAT Benchmark	F1-Score
Method 1: Zero-shot learning from MOF-KG ontology only. Prompt ChatGPT with the MOF-KG ontology definitions. Instruct ChatGPT to translate a user question to a Cypher query based on the ontology.	0.411
Method 2: 1-shot learning from a pair of train question and query. Using the embeddings of the test and train questions to find the most similar train question to the test question. Prompt ChatGPT with the pair of matched train question and query. Instruct ChatGPT to translate a test question to a Cypher query.	0.829
Method 3: 1-shot learning from the MOF-KG ontology and a pair of train question and query. As in Method 2, include MOF-KG ontology in the prompt, in addition to a pair of matched question and query.	0.845
Method 4: 1-shot learning from a pair of train question and query, and the chain-of-thought of the train query. As in Method 2, include the chain-of-thought of the train query in the prompt, in addition to the pair of matched question and query	0.876
Method 5: 1-shot learning from the MOF-KG ontology and a pair of train question and query, and the chain-of-thought of the train query. As in Method 3, include the chain-of-thought of the train query in the prompt, in addition to MOF-KG ontology and the pair of matched question and query.	**0.891**

Table 1: Evaluation results of leveraging ChatGPT to convert natural language questions to Cypher queries on the KGQA4MAT benchmark

effectively translates natural language questions into Cypher queries, achieving a high F1-score of 0.891 when the ontology, a matched pair of <question, query> as a training example, and a set of logical steps in a chain-of-thought explanation about the training query are provided.

7.2 Evaluation on QALD-9 Dataset

We also evaluate the performance of the proposed approach leveraging ChatGPT for KGQA on the QALD-9 [12] dataset, which contains natural language questions and corresponding SPARQL queries over DBpedia. QALD-9 is a multilingual question answering benchmark containing 408 train questions and 150 test questions. We only evaluate its English version of train and test questions. As a pre-trained large language model, ChatGPT has been trained on a variety of text sources, including Wikipedia. Consequently, when assessing ChatGPT on the QALD-9 dataset, we did not specifically incorporate the concept and relationship definitions from the DBpedia ontology in the prompts, assuming that ChatGPT has already learned the ontology.

Translated SPARQL queries are executed on the current DBpedia SPARQL endpoint[7]. Subsequently, we compare the results with those obtained from the correct SPARQL query to determine the accuracy of a translated query. The performance is measured using precision, recall, and F1-score, as previously defined in equations (1), (2), and (3).

Table 2 shows the evaluation results in comparison to the best performance in the KGQA leaderboard on QALD-9[8] as of April, 2023. The results show that the proposed approach that leverages ChatGPT can successfully translate natural language questions into SPARQL queries with a competitive performance compared to other state-of-the-art approaches.

[7]https://dbpedia.org/sparql
[8]https://github.com/KGQA/leaderboard/blob/gh-pages/dbpedia/qald.md#qald-9

Evaluation Method on the QALD-9 Benchmark	F1-Score
Baseline 1: SGPT_Q,K, 2022, top 1 in the KGQA Leaderboard as of April 2023 [27]	0.67
Baseline 2: SGPT_Q, 2022, top 2 in the KGQA Leaderboard as of April 2023 [27]	0.60
Baseline 3: Stage I No Noise, 2022, top 3 in the KGQA Leaderboard as of April 2023 [45]	0.55
Baseline 4: GPT-3.5v3, 2023, top 6 in the KGQA Leaderboard as of April 2023 [32]	0.46
Baseline 5: ChatGPT, 2023, top 7 in the KGQA Leaderboard as of April 2023 [32]	0.45
Method 0: Answer the QALD-9 questions directly. Instruct ChatGPT to answer the QALD-9 questions directly	0.33
Method 1: Translate QALD-9 questions directly. Instruct ChatGPT to translate QALD-9 questions directly, and then query DBpedia using the translated queries.	0.3
Method 2: 1-shot learning from a pair of train question and query. Using the embeddings of the test and train questions to find the most similar train question to the test question. Prompt ChatGPT with the pair of matched train question and query. Instruct ChatGPT to translate a test question to a SPARQL query over DBpedia.	0.40
Method 3: 1-shot learning from a pair of train question and query, and the chain-of-thought of the train query. As in Method 2, include the chain-of-thought of the train query in the prompt, in addition to the pair of matched question and query	**0.66**

Table 2: Evaluation results of leveraging ChatGPT to convert natural language questions to SPARQL queries on the QALD-9 benchmark

8 Discussion

Our results demonstrate the potential of using ChatGPT to translate natural language questions to knowledge graph queries. As seen in the evaluation, the highest F1-score of 0.891 is achieved when the ontology, a matched pair of <question, query> as a training example, and a set of logical steps in a chain-of-thought explanation about the query are provided. Comparing the performance of ChatGPT on MOF-KG and QALD-9 datasets, we observe that our approach is generalizable and can be adapted to different knowledge domains. However, there is a significant gap between the best performance on MOF-KG (F1-score=0.891) and the best performance on QALD-9 (F1-score=0.66). One possible reason is the different sizes of the ontologies describing the two knowledge graphs. The MOF-KG ontology only has 26 concepts and relationships, while the DBpedia ontology currently covers 685 classes and 2,795 different properties[9]. In our experiments, we relied on the ChatGPT's internal knowledge about the DBpedia ontology to translate users' questions. Despite utilizing only a single pair of <question, query> as a training example with a chain-of-thought explanation, ChatGPT managed to achieve performance comparable to the leading systems on the current KGQA leaderboard. These top systems typically employ sophisticated data processing strategies and advanced deep-learning models.

We carefully analyzed the natural language (NL) questions for which ChatGPT made errors when translating them into knowledge graph (KG) queries. We observed that the primary mistakes occurred when ChatGPT failed to utilize the correct path within the knowledge graphs, including alternative paths. For example, ChatGPT displayed a tendency to generate new concepts and properties in the KG queries, even though we explicitly incorporated the following instruction in the prompt: "*only use the concepts and relationships in the given ontology.*" The another example is the 'UNION' operation that combines multiple alternative paths. ChatGPT could not correctly apply 'UNION' in many cases. Here are some examples to further illustrate these issues.

[9]http://wikidata.dbpedia.org/services-resources/ontology

Example from the KGQA4MAT Benchmark:

Question: What is the total number of operation conditions of all synthesis operations for any MOFs ‘MIL-53’?

Training Question: What is the overall count of operation conditions for all the synthesis procedures associated with any MOFs ‘MOF-3’?

Training Query: MATCH (m:MOF)-[:has_publication]->(:Publication) <- [:has_publication]-(s:Synthesis_Procedure)-[:has_operation]-> (o:Synthesis_Operation)- [:has_condition]-> (c:Synthesis_Operation_Condition) WHERE m.name CONTAINS ‘MOF-3’ RETURN count(c);

ChainOfThought: {logical steps in the training query. Check the detailed chain of thought steps in the training data set.}

Correct Query: MATCH (m:MOF)-[:has_publication]->(:Publication) <-[:has_publication]-(s:Synthesis_Procedure)-[:has_operation]-> (o:Synthesis_Operation)-[:has_condition]-> (c:Synthesis_Operation_Condition) WHERE m.name CONTAINS ‘MIL-53’ RETURN count(c)

<u>**Incorrect Answer:**</u> MATCH (m:MOF)-[:has_synthesisProcedure]-> (sp:Synthesis_Procedure)-[:has_operation]->(o:Synthesis_Operation) -[:has_condition]->(c:Synthesis_Operation_Condition) WHERE m.name CONTAINS ‘MIL-53’ RETURN count(c);

Issues: Despite the training question being highly similar to the question being asked, with the correct query differing only in the MOF identification, ChatGPT still made an error in the translation process. It is important to note that ChatGPT was provided with chain-of-thought logical steps in the training query to facilitate its understanding. However, the model still introduced an invented relationship (m:MOF)-[:has_synthesisProcedure]->(sp:Synthesis_Procedure), which ultimately led to an incorrect answer.

Example from the QALD-9 Benchmark:

Question: Which countries in the European Union adopted the Euro?

Training Question: Which countries adopted the Euro?

Training Query:

```
SELECT DISTINCT ?uri
WHERE {
?uri a <http://dbpedia.org/ontology/Country>
{ ?uri <http://dbpedia.org/ontology/currency>
<http://dbpedia.org/resource/Euro> }
UNION
{ ?uri <http://dbpedia.org/property/currencyCode> "EUR"@en }
```

ChainOfThought: {logical steps in the training query. Check the detailed chain of thought steps in the training data set.}

Correct Query:
```
SELECT DISTINCT ?uri
WHERE { ?uri a <http://dbpedia.org/ontology/Country>
{ ?uri <http://dbpedia.org/ontology/currency>
<http://dbpedia.org/resource/Euro> }
UNION
{ ?uri <http://dbpedia.org/property/currencyCode> "EUR"@en } }
```

Incorrect Answer:
```
PREFIX rdf:  <http://www.w3.org/1999/02/22-rdf-syntax-ns#>
PREFIX rdfs:  <http://www.w3.org/2000/01/rdf-schema#>
PREFIX dbo:  <http://dbpedia.org/ontology/>
PREFIX dct:  <http://purl.org/dc/terms/>
PREFIX dbp:  <http://dbpedia.org/property/>
SELECT DISTINCT ?country
WHERE { ?country a dbo:Country ;
dct:subject <http://dbpedia.org/resource/Category:
Member_states_of_the_European_Union> .
?country dbo:currency <http://dbpedia.org/resource/Euro> .  }
```

Issues: The training question closely resembles the test question, with the training query involving a 'UNION' operation that combines two alternative paths. Despite the chain-of-thought steps providing instructions for the 'UNION' operation, ChatGPT failed to generate the correct query, resulting in a missing 'UNION' operation.

These examples demonstrate the challenges that needs to be addressed in order to improve the approach of utilizing ChatGPT in generating accurate KG queries from NL questions.

9 Conclusion

We developed a benchmark dataset for Knowledge Graph Question Answering for Materials Science (KGQA4MAT) and a systematic approach for utilizing ChatGPT to translate natural language questions into formal KG queries. Our evaluation demonstrated the potential of utilizing ChatGPT for addressing KGQA issues across different platforms and query languages. The MOF-KG, KGQA4MAT benchmark, and the proposed approach facilitate further development on user-friendly interfaces enabling domain experts to more easily access and interrogate the wealth of information contained within materials science knowledge graphs. Future research directions include refining the proposed approach, expanding the benchmark dataset, and exploring alternative techniques for KGQA in the context of materials science.

9.0.1 Benchmark Repository.

The benchmark data, MOF-KG definitions, ChatGPT prompts, Python code for evaluation are accessible via the following GitHub repository: https://github.com/kgqa4mat/KGQA4MAT[10] .

9.0.2 Acknowledgments.

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[10]https://github.com/kgqa4mat/KGQA4MAT

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