SCIENCE HIERARCHOGRAPHY: Hierarchical Organization of Science Literature

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Abstract

Scientific knowledge is growing rapidly, making it difficult to track progress and high-level conceptual links across broad disciplines. While tools like citation networks and search engines help retrieve related papers, they lack the abstraction needed to capture the *density* and structure of activity across subfields.

We motivate SCIENCE HIERARCHOGRAPHY, the goal of organizing scientific literature into a high-quality hierarchical structure that spans multiple levels of abstraction—from broad domains to specific studies. Such a representation can provide insights into which fields are well-explored and which are under-explored. To achieve this goal, we develop a hybrid approach that combines efficient embedding-based clustering with LLM-based prompting, striking a balance between *scalability* and *semantic precision*. Compared to LLM-heavy methods like iterative tree construction, our approach achieves superior quality-speed trade-offs. Our hierarchies capture different dimensions of research contributions, reflecting the interdisciplinary and multifaceted nature of modern science. We evaluate its utility by measuring how effectively an LLM-based agent can navigate the hierarchy to locate target papers. Results show that our method improves interpretability and offers an alternative pathway for exploring scientific literature beyond traditional search methods. [1]

1 Introduction

The pace of scientific publishing is accelerating (Ware and Mabe, 2015), but this growth is uneven across fields (Hope et al., 2023). Some areas attract dense research activity, while others remain underexplored. This raises a natural question:

> *How do we understand the* <u>*distribution*</u> *of scientific efforts across different sub-areas?*

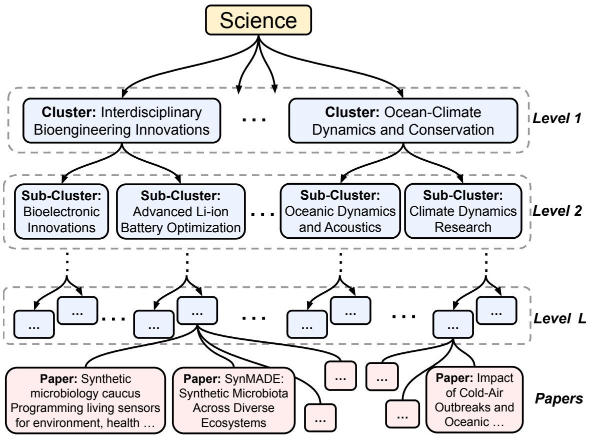
Science
Cluster: Interdisciplinary Bioengineering Innovations
...
Cluster: Ocean-Climate Dynamics and Conservation
Level 1
Sub-Cluster: Bioelectronic Innovations
Sub-Cluster: Advanced Li-ion Battery Optimization
...
Sub-Cluster: Oceanic Dynamics and Acoustics
Sub-Cluster: Climate Dynamics Research
Level 2
...
Level L
Paper: Synthetic microbiology caucus Programming living sensors for environment, health …
Paper: SynMADE: Synthetic Microbiota Across Diverse Ecosystems
Paper: Impact of Cold-Air Outbreaks and Oceanic …
Papers

Figure 1: An example of SCIENCE HIERARCHOGRAPHY illustrates how scholarly work can be organized hierarchically—from broad research domains at the top, through increasingly specific sub-clusters, down to individual papers at the lowest level. Critically, this structure must be inferred automatically and at scale.

Answering this question is essential *for both academic and policy stakeholders*. A clearer view of how research efforts are distributed enables institutions to spot emerging or neglected areas, prioritize strategic hiring and future agendas. For policymakers, it supports more informed funding decisions, ensuring that critical but underexplored domains receive the attention and resources they deserve.

Conventional tools like Google Scholar are designed as retrieval engines, optimized to return a handful of papers that match a specific query. They offer little in the way of a comprehensive or structured view of the broader scientific landscape. Similarly, while modern LLM-based assistants can surface related works (seen during pretraining or via their retrieval tools), they fall short in offering a broad, bird's-eye perspective on scientific progress.

Addressing this challenge requires abstraction: a way to generalize over research problems and techniques and to connect broad scientific areas to specific papers via intermediate categories. At one end, we have high-level domains (e.g., physics, AI); at the other, individual papers. Between them lie a latent spectrum of subfields and methodological

[1] Code, data and demo are available: `https://github.com/JHU-CLSP/science-hierarchography`

clusters. What's missing is a data structure that captures all these abstraction levels.

We propose building large-scale hierarchical representations of scientific literature, which we call SCIENCE HIERARCHOGRAPHY. A well-designed hierarchy provides a macro-level view of scientific progress, revealing how research is distributed across methods and application areas. This helps researchers spot emerging trends and gaps, and supports policymakers and institutions in making more strategic resource decisions. It also offers a new way to explore the literature—complementing traditional search by allowing users to navigate science through conceptual hierarchies.

How should scholarly work be represented? A central challenge in building a scientific hierarchy is defining what each node represents. Research papers often span multiple topics (e.g., *reinforcement learning for medical imaging* or *deep learning for oceanography*). To capture this complexity, we develop a prompting strategy that decomposes papers into key *contribution* types—such as the *problems addressed* and *techniques used* (§3.2). For each fixed contribution type, we construct a corresponding hierarchical structure, ensuring that papers are organized into meaningful, coherent categories.

What construction strategies balance scalability and quality? To address this, we introduce SCYCHIC (pronounced "psychic"), a new method for building high-quality hierarchical structures of scientific literature. SCYCHIC integrates fast embedding-based clustering with LLM prompting, combining the efficiency of embeddings with the semantic precision of language models (§4.1).

How can we evaluate the quality of a scientific hierarchy? Scientific hierarchies lack a fixed ground truth—they evolve over time as research landscapes shift. We therefore adopt an *evaluation-through-utilization* approach, measuring *whether an information seeker (human or AI) can efficiently locate specific content* (e.g., child nodes) by navigating the hierarchy from the root. This evaluation hinges on the idea that a good hierarchy enables rapid information discovery, even though its utility extends well beyond search alone (§5.2).

What did our empirical results show? Our approach achieves the best trade-off between quality and speed when compared to LLM-heavy methods like iterative tree construction or pruning. Extensive experiments show that SCYCHIC consistently produces higher-quality hierarchies than a broad set of baselines (§5.4). Validation on a 10K-paper dataset further confirms its strong accuracy and scalability for large-scale use.

Contributions: (1) We introduce the goal of constructing large-scale, abstract hierarchies of scientific literature to reveal how scholarly efforts are distributed across research areas. (2) We propose a utilization-based evaluation framework that measures how effectively users can discover information by traversing the hierarchy. (3) We present SCYCHIC, a new method that combines fast embedding-based clustering with LLM prompting to build high-quality, multidimensional hierarchies. Extensive experiments show that SCYCHIC outperforms baseline approaches, offering a more structured and bird's-eye view of scientific progress.

2 Related Work

Gierarchy induction: The field of taxonomy induction has progressed from early pattern-based techniques to modern LLM-augmented methods. Seminal work by Hearst (1992) introduced the use of hand-crafted hyponym patterns for extracting is-a relationships. Subsequent research expanded on this using statistical methods and large-scale information extraction to identify hypernym-hyponym structures (Pantel and Pennacchiotti, 2006; Yang and Callan, 2009; Girju et al., 2006).

Recent advances incorporate LLMs prompting to enhance taxonomy construction. For example, Wan et al. (2024); Zeng et al. (2024a); Chen et al. (2023); Zeng et al. (2024b) apply zero-/few-shot reasoning and ensemble ranking, while others explore open-ended, vocabulary-free taxonomy creation (Gunn et al., 2024), self-supervised expansion in low-resource domains (Mishra et al., 2024), and graph-based methods leveraging metadata and citations (Cong et al., 2024; Sas and Capiluppi, 2024; Shen et al., 2024). Optimization and in-context learning have also shown promise (Hu et al., 2024b; Shi et al., 2024; Xu et al., 2025; Jain and Espinosa Anke, 2022; Chen et al., 2021).

Our work differs in scope, scale, and methodological design. We focus on scaling taxonomy induction for the domain of scholarly literature—a setting that presents greater challenges than typical setups (e.g., entity hierarchy) due to the complexity, size, and evolving nature of scientific content. The most comparable effort is by Oarga et al. (2024), though our broader objectives require fundamentally different algorithmic strategies and operate without access to ground truth labels.

System	# of Levels	Node content	Node granularity	Assigned by	Purpose	Public
Web of Science	One	Research areas	One keyword	Publisher	Indexing	No
Scopus	Two	Research areas	One keyword	Editor	Indexing	Yes
arXiv Taxonomy	Two	Research areas	One keyword	Authors	Indexing	Yes
PubMed MeSH	Multiple	Medical headings	One keyword	Authors	Indexing	Yes
Microsoft Academic Graph	Multiple	Research areas	Multiple keywords	Algorithms	Indexing	Discontinued
SCIENCE HIERARCHOGRAPHY (Ours)	Multiple (by designer)	Rich contribution descriptions	Science contribution summary (many tokens)	Algorithms	Exploratory Analysis	Yes

Table 1: Comparison of hierarchical resources for organizing scientific literature, ordered by hierarchy depth. Conventional systems are built for indexing, relying on fixed, shallow taxonomies with keyword-based nodes and human-assigned labels. In contrast, SCIENCE HIERARCHOGRAPHY supports deeper, designer-controlled hierarchies with rich natural-language summaries, enabling more flexible and exploratory analysis of scientific work.

Structured representation of science: As science grows at an unprecedented rate (Teufel et al., 1999; Pertsas and Constantopoulos, 2017; Constantin et al., 2016; Fisas et al., 2016; Liakata et al., 2010), numerous frameworks have emerged to structure this information through knowledge graphs and taxonomies (Fathalla et al., 2017; Jaradeh et al., 2019; Oelen et al., 2020; Vogt et al., 2020; Soldatova and King, 2006). Recent work includes prompt-based topic modeling (Pham et al., 2024), iterative taxonomy construction that incorporates object properties and graph mining (Cui et al., 2024; Marchenko and Dvoichenkov, 2024), and hybrid approaches that combine curated ontologies with data-driven maps (Zimmermann et al., 2024). Our work builds on these efforts by constructing a high-quality hierarchical structure tailored to scientific literature, in three key ways. The prior work: (1) Produces shallow hierarchies, typically only one or two levels deep; (2) Uses cluster labels based on keywords, whereas ours are derived from natural language summaries of papers; (3) Depends heavily on manual effort, while our pipeline is fully automated.

In Table 1 we summarize the differences with existing hierarchical resources. While most prior systems are limited to one/two level(s) of depth and rely on manually assigned labels for indexing—a process often prone to bias (Hadfield, 2020)—our approach supports deeper, algorithmically generated hierarchies with semantically rich node descriptions. This enables a more flexible and interpretable representation of scientific knowledge.

3 SCIENCE HIERARCHOGRAPHY: Toward Hierarchy of Scholarly Work

We begin with a formal problem definition (§3.1), followed by content representation (§3.2) and depth considerations (§3.3).

3.1 Formal Problem Statement

We define the task of SCIENCE HIERARCHOGRAPHY as an inference problem where the **input** is a large set of scientific papers: $P = \{p_1, p_2, \ldots, p_n\}$. The goal is to infer a hierarchical structure for these papers (e.g., their problems and techniques). This structure represents levels of specificity and abstraction, with nodes closer to the root representing broader topics. Broader topics are at the upper levels, while more specific subtopics and individual papers are at the lower levels.

Formally, this goal is defined as inferring a graph that encodes relationships between nodes (atomic concepts representing scholarly ideas or goals). This is formally defined as $T := (N, E)$ where:

- N is the set of all concepts (nodes) present in the hierarchy: $N = \{n_1, n_2, \ldots, n_N\}$.
- E is the set of all edges connecting node pairs: $E = \{r_1, r_2, \ldots, e_M\}$ where each edge is a node pair $r_i = (n_p, n_c)$ connects a parent node n_p to its child node n_c.
- For each edge $e \in E$, there is a type attribute: $\text{type}(e) \in \{\text{“isA”}, \text{“instanceOf”}\}$ associated with the edge.
- Each node $n \in N$ has a property $n.prop$ which defines the content of the node (e.g., a sentence description or a few keywords).

The edge (relations connecting two nodes) have types that is either “isA” relationships or “instanceOf.” The "isA" relationship defines a hierarchical link between node pairs, indicating a child node is a subclass of its more abstract parent node (e.g., "RLHF isA RL" means "RLHF" is a type of "RL"). The "instanceOf" relationship indicates that a specific instance belongs to a concept category (e.g., "Ouyang et al. (2022) instanceOf RLHF" means "Ouyang et al. (2022)" is a specific instance of the broader “RLHF” cluster).

3.2 Decomposing Papers to Contributions

A central challenge is how to represent the content of scholarly work within hierarchy nodes. Scientific papers are idea-dense, often combining broad goals, specific problems, and technical methods. To capture this complexity, we extract structured representations that disentangle these distinct aspects (D'Souza and Auer, 2020). This also mitigates the issue of input length: papers typically range from 4 to 10 pages (5K to 10K tokens), making full-document processing across large corpora infeasible and costly for LLMs.

We use an LLM to preprocess each paper (title and abstract) and break them down into a **predefined set of contributions**, akin to prior work (Hope et al., 2017; Chan et al., 2018) that mine "problem schema" from existing documents. We consider the following contribution types: (1) **problem statement** (the problem addressed), (2) **solution** (the technical approach used), (3) **result** (the key finding), and (4) **topic** (the overarching themes). (See §C for prompts and examples). We note that each contribution may include additional dimensions (sub-contributions). For instance, a "result" encompasses both the "outcome" and its "potential impact."

3.3 Choosing Hierarchy Depth

While the ideal number of hierarchy layers is ultimately empirical, we can build useful intuition from the structure of a near-balanced tree. For a tree with branching factor b and depth L, the total number of nodes is roughly $O(b^L)$. To organize C contributions, the number of nodes should scale with C, implying a depth of $L = O(\log_b C)$. In practice, we use $L = 3$ for a 2K-paper corpus and $L = 4$ for 10K papers, consistent with this logarithmic scaling. Extrapolating further, corpora of 10^7 papers would likely require depths of $L = 6$ or 7.

4 Tackling SCIENCE HIERARCHOGRAPHY

We present algorithms to address our proposed goal. We start with our main method, SCYCHIC (§4.1), explore its special cases (§4.2), and then describe alternative baselines that rely more heavily on LLMs (FLMSCI; §4.3). While all approaches leverage LLMs to some extent, they differ significantly in their reliance on them: some require many calls (linear or quadratic in the number of papers), while others are more efficient (e.g., logarithmic). Since our goal is to scale to millions of papers, minimizing LLM usage is critical. Our objective is to identify the method that yields the highest-quality hierarchy with the lowest LLM overhead, balancing quality, latency, and cost.

4.1 SCYCHIC: Alternating Between Clustering and Summarization

This approach is based on the following design choices: (1) access to `embedder`, a neural model that converts a description into a d-dimensional vector, (ideally) capturing its semantic meaning; (2) a clustering algorithm `clusterer` that, given the hyperparameter k, generates k clusters; (3) a contribution type (e.g., problem definition) and its dimensions C extracted per paper as detailed in §3.2 which determines the focus of the node descriptions; (4) `summarizer`, an LLM that generates a summary description which (ideally) provides a more abstract description of a collection of node descriptions; and (5) the total number of hierarchy layers L and target number of clusters in each layer $(k_1, k_2, \ldots, k_L)$.

Initialization: The approach begins by embedding each papers. For each paper p_i, we embed each component in C: $\texttt{embedder}(c^i_j) \in \mathbb{R}^d$, where $j \in C$. This process results in $|C|$ embeddings per paper. We concatenate these embeddings, yielding $\mathbb{R}^{d.|C|}$ embeddings per paper. With this, we present the main algorithm which involves two phases:

Top-down phase: First, we use a **top-down** strategy, iterating through the top half of the layers. For each layer $l \in (1 \ldots \lfloor L/2 \rfloor)$ (starting from the root and moving downward), we cluster the documents using `clusterer`.

For the first layer ($L = 1$), we partition the entire paper collection into k_1 top-level clusters using their embeddings. For the second level, we process each top-level cluster independently, i.e., within each top-level cluster, we take only the papers belonging to that cluster and apply `clusterer` to their embeddings to divide them into subgroups.

This process continues recursively: for subsequent layers, clustering operates on the data points within each cluster. We run as many clustering algorithms as there are clusters in the previous layer. The allocation of the total cluster count across different top-level clusters is determined proportionally based on the number of papers in each top-level cluster. If a top-level cluster contains a larger proportion of papers, it will be allocated more subclusters from the total cluster count. This proportional allocation ensures that areas with higher paper density receive finer-grained clustering.

This recursively subdivides each cluster at level l into multiple clusters at level $l+1$. This top-down phase continues until we reach level $\lfloor L/2 \rfloor$. Alongside clustering, we also use the summarizer to generate abstracted summaries for each of the clusters. The generated cluster description follows the same structure or style as the input descriptions. For example, if the inputs are statements about problem categories, the output from summarizer is also in the same style, but more abstract.

Bottom-up phase: In the second phase, we switch to a **bottom-up** strategy to construct the remaining levels ($\lfloor L/2 \rfloor + 1$ through L). To form clusters for bottom-level (layer L), we apply clusterer to the paper embeddings within each sub-cluster within level-$\lfloor L/2 \rfloor$ (the lowest level clustering obtained from top-down approach). We then use the summarizer to create an abstracted description for each cluster.

We repeat this process for all layers from L to $\lfloor L/2 \rfloor + 1$. To build layer l, we start by embedding the generated cluster summaries from the level below $l-1$ using embedder, similar to how we embedded the papers. We then run the clustering clusterer on these new embeddings and generate abstracted summaries for the clusters to group these summaries into higher-level clusters. This bottom-up aggregation continues until we connect with the previously constructed level $\lfloor L/2 \rfloor$ clusters.

Algorithm 1 SCYCHIC algorithm

```
Require: Set of papers $P = \{p_1, p_2, \ldots, p_n\}$, embedder, clusterer, summarizer, num of layers $L$, target cluster sizes $(k_1, k_2, \ldots, k_L)$
Initialization: For each paper $p_i \in P$, embed their selected components to form $\mathbb{R}^{d \times |C|}$.
for layer $l = 1$ to $\lfloor L/2 \rfloor$ do                    ▷ Top-down phase
    if $l = 1$ then
        Apply clusterer to divide papers into $k_1$ clusters
    else
        for each cluster from layer $l - 1$ do
            Apply clusterer to divide into subclusters
    Use summarizer to generate summaries for each cluster
for each cluster $\kappa$ at level $\lfloor L/2 \rfloor$ do        ▷ Bottom-up phase
    for layer $l = L$ to $\lfloor L/2 \rfloor + 1$ do
        if $l = L$ then
            Collect the embeddings of papers within $\kappa$.
        else
            Apply embedder on summaries of cluster $l+1$
        Apply clusterer to form higher-level clusters
        Use summarizer to generate abstracted summaries
return Hierarchical structure
```

Rationale behind the hybrid design: The hybrid approach merges the strengths of top-down and bottom-up strategies. A bottom-up method may create less coherent top-level clusters. The top-down approach ensures high-quality top-level clusters but doesn't utilize the abstracted summaries from summarizer used by bottom-up clustering. By combining both methods, the hybrid design achieves robust and effective clustering. Our empirical results in §5.4 demonstrate this approach's strength by balancing quality and scalability.

4.2 Top-down and Bottom-up Baselines

We examine two special cases of SCYCHIC: one using only a top-down strategy and the other solely with a bottom-up approach. These variants help isolate and evaluate the strengths and limitations of each method. Results are discussed in §5.4.

4.3 Pure LLM-based Baselines

We introduce baselines that heavily utilize LLM calls, based on the hypothesis that LLMs can make high-quality local decisions, collectively forming a robust global structure. The potential cost here is the need to make *many* LLM calls. We refer to these baselines as FLMSCI (pronounced "flimsy") and present two variants below.

Initializing a Seed Hierarchy: The first step involves creating a seed hierarchy, starting with the hierarchy of sciences from the Wikipedia page on branches of science.[2] We made several adjustments to this hierarchy, detailed in §D, where the resulting seed hierarchy is also included.

FLMSCI (parallel): Adding Many Items in Parallel with Few Prompts: This approach involves adding items to the seed hierarchy in parallel. First, gather all unique items extracted from different papers and create batches of 100 items each (batching because all of these items would not fit within the context window of LLM). Then, implement a multi-threaded program where each thread adds a batch of keywords to a clone of the seed hierarchy. Finally, merge (with a Python program, not an LLM call) all these cloned trees into a single comprehensive structure.

FLMSCI (incremental): Expand the tree by incrementally adding items one at a time: This approach involves an iterative, layer-by-layer prompt that navigates the tree starting from the root node and performs specific actions. By default, the supported actions include: (a) *Go down*: select one

[2] en.wikipedia.org/wiki/Branches_of_science

of the nodes to traverse down to a lower layer in the tree; (b) *Add sibling*: Insert a new node at the same level; (c) *Make parent*: Create a new parent node; (d) *Discard*: Ignore the item, if no suitable location is found. This prompt are shown in Fig.11.

The available actions vary depending on the tree's current position. To prevent placing detailed items too high in the tree (above layer 3), we hide the actions that involve nodes (b) and (c). This restriction provides more control and reduces errors, as observed in pilot experiments. If the traversal reaches a child node, we hide the option to move further down (a). Another issue identified was frequent mistakes in earlier layers, likely due to broad labels where multiple categories could fit. To address this, we provide more context for the first layer by replacing label strings with descriptive definitions, as shown in Fig.10.

4.4 Computational Complexity of Approaches

A major scalability bottleneck in hierarchy construction is the number of LLM calls. Let C be the number of contributions (§3.2), b the branching factor, and $L = O(\log_b C)$ the maximum depth for a near-balanced tree (§3.3). Our proposed algorithm, SCYCHIC, requires $O(C/b)$ LLM calls for both its top-down and bottom-up variants. Among the LLM-based baselines discussed in §4.3, FLMSCI (parallel) makes $O(C/l)$ calls (with l as batch size), offering lower complexity but at the cost of reduced quality. In contrast, FLMSCI (incremental) achieves higher accuracy but requires $O(C \log_b C)$ LLM calls due to root-to-leaf traversals during insertion. Empirically, the difference in LLM usage is significant: in our 2K-paper setup, FLMSCI (incremental) makes 61K calls compared to just 322 for SCYCHIC (Table 3).

Approach	# of LLM calls
SCYCHIC	$O(C/b)$
FLMSCI (parallel)	$O(C/l)$
FLMSCI (incremental)	$O(C \log_b C)$

Table 2: Computational complexity of hierarchy construction methods measured by LLM calls, with C = contributions, b = branching factor, and l = batch size.

5 Experimental Setup and Results

We describe our experimental setup, including the diverse paper collection used for our experiments (§5.1) and the evaluation framework (§5.2).

5.1 Collection of Science Papers

We compile a collection of scientific papers spanning domains such as computer science, neuroscience, biology, oceanography, and their interdisciplinary intersections. Our initial analysis focuses on a smaller set of approximately $2K$ papers (referred to as **SciPile**), allowing for rapid iteration over design choices and assessment of scalability. We then extend our analysis to a larger collection of $10K$ papers, referred to as **SciPileLarge**. Details on data collection and filtering are provided in §F.

5.2 Evaluation as Utilization

Ideally, hierarchy quality would be evaluated against a gold standard—but no such reference exists, and scientific literature continually evolves. As a result, we adopt an evaluation framework based on *utilization*, independent of fixed ground truth.

We assess hierarchy quality by measuring *how well it supports navigation and content discovery*. Specifically, we use an LLM-based agent to locate target papers via tree traversal, tracking accuracy at each level and across the full hierarchy. A stronger hierarchy should better capture conceptual relationships and improve information-seeking efficiency. While our evaluation focuses on retrieval, the hierarchy's utility extends beyond that.

Two key design choices guide our evaluation: (a) selecting appropriate queries, and (b) choosing a reliable LLM. For (a), we sample paper titles and abstracts as queries. Although we considered generating language questions from papers, pilot studies showed both approaches yield similar results, so we use the simpler method. For (b), we use `Qwen2.5-32b-instruct`, which demonstrated performance closest to GPT-4 among open models in our pilot evaluations (§B).

Starting at the top of the hierarchy, we provide the evaluator (LLM) with the query and the list of cluster descriptions (prompt in Fig. 2). The model must select the cluster it deems most relevant. We move to the next level only if the chosen cluster contains the target paper. At each subsequent level, the same query is used, but only subclusters of the previously selected (and correct) cluster are shown. This continues until the model reaches the level containing the target paper. We report two metrics: Strict Accuracy (**Strict-Acc**), which captures how often the model selects the exact correct node, and Layer-1 Accuracy (**L1-Acc**), which measures how often it selects the correct top-level subtree.

Method	Strict-Acc (%) ↑	L1-Acc (%) ↑	# of Calls ↓
Topic contributions			
SCYCHIC	**14.9** ± 2.7	**65.7** ± 4.4	322
↳Top-down	14.5 ± 4.7	62.5 ± 7.4	322
↳Bottom-up	13.9 ± 5.3	54.4 ± 12.7	322
↳FLMSCI (par)	4.0 ± 2.8	32.0 ± 6.3	226
↳FLMSCI (inc)	**18.0 ± 5.3**	**91.0 ± 4.0**	**61K**

Table 3: Evaluations results for SCYCHIC, FLMSCI (**par**allel) and FLMSCI(**inc**remental) when using *Topic* as the contribution type. All methods exhibit low Strict-Acc ($\leq 18.0\%$), underscoring the difficulty of the task. While FLMSCI (inc) achieves the highest accuracy, it requires approximately 200× more LLM calls than other methods. In contrast, SCYCHIC strikes a balance between performance and efficiency, achieving competitive accuracy (14.9% Strict-Acc, 65.7% L1-Acc) with substantially lower computing cost. Full results in §H.1.

5.3 Experiment Design

We conduct few sets of experiments to evaluate our method (SCYCHIC, §4.1) against the baselines (§4.2, 4.3) following the proposed evaluation protocol. Hyperparameter details for SCYCHIC are provided in §G. The experiments are structured as follows: (1) We begin by comparing all methods on "topic" contributions, the simplest contribution type (Table 3). Due to the high computational cost, LLM-based baselines are evaluated only in this setting. (2) We then evaluate performance on more complex contributions (problem, solution, and results) using both **SciPile** and **SciPileLarge** to test scalability (Table 4). The results tables also report *LLM Cost* (average number of input tokens and LLM calls) and *Hierarchy Structure* (depth and branching factor per node).

5.4 Empirical Findings

SCYCHIC outperforms its special-case baselines. As shown in Table 3, SCYCHIC achieves higher Level-1 accuracy than the top-down and bottom-up baselines, while maintaining comparable Strict-Acc. Similar trends hold across other contribution types in Table 4. For example, on "solution" contributions, SCYCHIC exceeds the top-down baseline by 2.9% in Strict-Acc and 3.1% in L1-Acc, highlighting its effectiveness. Notably, these gains are achieved with a similar number of tokens and LLM calls, underscoring SCYCHIC's compute efficiency.

LLM-based baselines can be far more expensive than SCYCHIC. While FLMSCI slightly outperforms SCYCHIC in accuracy, it does so at the cost of a *massive* increase in LLM calls—making it impractical for large-scale use. As a result, despite its strong performance, FLMSCI (incremental) simply doesn't scale.

SCYCHIC scales to larger paper corpus. For our scalability experiments, we evaluated SCYCHIC on our larger $10K$ paper dataset **SciPileLarge**, using the *problem statement* contribution type. Due to the significant increase ($\times 5$) in corpus size, we implemented a 4-layer hierarchy instead of the 3-layer structure used previously. Notably, SCYCHIC achieved even higher L1-Acc (86.5%) on **SciPileLarge** compared to our smaller dataset **SciPile**. This improvement likely stems from the enhanced quality of our expanded dataset, which has more strict filtering mechanisms. While the Strict-Acc showed a minor decrease compared to results on **SciPile**, it remained at a satisfactory level. Collectively, these results provide compelling evidence that our method scales successfully to substantially larger paper corpora.

5.5 Additional Analyses

We briefly cover additional analyses that were omitted from the main text due to space constraints.

Detailed prompts significantly improve hierarchy quality. To demonstrate this, we compare two prompt types. The first is a "detailed" prompt—carefully curated with comprehensive instructions and reminders—which we use for all main experiments in this paper. The second is a "simplified" prompt containing only the core task description. The results confirm that the detailed prompt consistently and substantially outperforms the simplified version across all scenarios. More detailed results are in §H.3.

Embedding quality varies significantly across models. For the `embedder` mentioned in §4.1. We evaluated three models—Qwen's `gte-Qwen2-7B-instruct` (Li et al., 2023), OpenAI's `text-embedding-3-large`, and `text-embedding-ada-002`. The first two models perform similarly, whereas `text-embedding-ada-002` produces markedly weaker results. We select `gte-Qwen2-7B-instruct` for its strong balance of performance and its practical value as an open-weight model for reproducible research. The experimental results are in §H.2.

5.6 Sample Visualization of the Hierarchy

The reader might be curious to see the resulting hierarchies. In §I we show a slice of the final

Method	Accuracy (%)		LLM Cost		Hierarchy Structure		
	Strict-Acc ↑	L1-Acc ↑	Avg. # of Input Tokens ↓	# of Calls ↓	Depth	Avg. Branching Factor	Max. Branching Factor
Dataset: SciPile (2K papers)							
Contributions type: Problem Statement							
Scychic	**51.1 ± 3.8**	**81.7 ± 2.6**	2624	322	3	7.1	20
↳Top-down	49.0 ± 3.7	80.3 ± 2.7	2953				18
↳Bottom-up	45.9 ± 5.0	69.3 ± 8.1	2177				16
Contributions type: Solution Statement							
Scychic	**48.8 ± 6.1**	**82.3 ± 1.1**	2343	322	3	7.1	16
↳Top-down	45.9 ± 5.5	79.2 ± 3.4	2521				19
↳Bottom-up	36.7 ± 2.6	67.0 ± 4.3	1990				14
Contributions type: Results Statement							
Scychic	46.4 ± 5.2	76.4 ± 6.9	2654	322	3	7.1	16
↳Top-down	**47.3 ± 3.1**	**80.5 ± 4.4**	2718				16
↳Bottom-up	40.0 ± 10.7	64.0 ± 8.9	2210				13
Dataset: SciPileLarge (10K papers)							
Contributions type: Problem Statement							
Scychic	**43.7 ± 6.5**	85.8 ± 4.2	7451	1572	4	8	26
↳Top-down	41.5 ± 8.2	**86.5 ± 5.6**	8990				30
↳Bottom-up	26.2 ± 5.4	41.9 ± 4.0	5924				26
Contributions type: Solution Statement							
Scychic	**24.7 ± 4.8**	**65.8 ± 2.5**	7653	1572	4	8	28
↳Top-down	22.4 ± 3.5	52.3 ± 3.0	4032				26
↳Bottom-up	23.9 ± 3.3	51.3 ± 3.1	6150				28
Contributions type: Results Statement							
Scychic	**27.6 ± 4.6**	**69.8 ± 2.1**	6457	1572	4	8	30
↳Top-down	19.7 ± 4.0	54.0 ± 3.3	5380				30
↳Bottom-up	23.6 ± 2.7	55.2 ± 2.9	4731				28

Table 4: Evaluation results of Scychic and the corresponding baselines on both the 2K (**SciPile**) and 10K (**SciPileLarge**) datasets. Scychic maintains high accuracy and a relatively small variance, proving the rationale behind our hybrid design. When scaling from 2K to 10K papers, our method shows a slight decrease in Strict-Acc but maintains strong L1-Acc, demonstrating its feasibility on larger datasets. Across both scales, the *problem statement* contribution type consistently yields the most accurate hierarchies, indicating this contribution type contributes most for hierarchy construction.

hierarchy generated by Scychic on the **SciPile-Large** dataset. The original hierarchy has 4 levels, use papers' *problem* contribution. Due to space constraints, this slice shows only two levels of clusters above the individual papers.

6 Discussion and Conclusion

Future applications: Our work opens several promising directions for future research. One key opportunity is to use the constructed hierarchies as tools for exploratory analysis across scientific domains. They can aid academic institutions and funding bodies in identifying emerging trends and underexplored areas, and can be adapted for domain-specific analyses that capture the unique structure of individual fields. This approach not only deepens our understanding of scientific progress but also provides a new lens for organizing the vast and growing body of scholarly work.

Conclusions: We introduced Science Hierarchography, a framework for large-scale hierarchical summarization of scientific literature, offering a new lens on how research efforts are distributed. Our method, Scychic, combines LLMs with efficient algorithms to strike a balance between quality and scalability. Looking forward, we aim for this work to help researchers navigate the scientific landscape more intuitively and support more informed resource allocation in academia.

Limitations

Although we evaluated our pipeline on $10K$ papers, this is still far from the true scale of scientific literature. We hope future work will enhance our approach to handle more realistic scales. Additionally, while our evaluation framework shows potential for efficient information discovery, it may have its own weaknesses and biases. Integrating human verification into the assessment process could help ensure the quality and reliability of the inferred hierarchies.

Ethics Statement

In our work, all data and models are accessed via licenses that grant us free and open access for research purposes. Expert annotations are provided by the paper's authors, who have contributed their efforts without compensation. We have not observed any harmful content in either the scholarly papers or the content generated by LLMs. On the other hand, since our resulting hierarchy reflects the distribution of scientific efforts across various fields, it offers a detailed map of where research activity is concentrated and where it is lacking. This nuanced view can guide decision-makers—such as government agencies and academic institutions—in making more informed choices about resource allocation. By highlighting underexplored yet promising areas alongside well-established fields, the hierarchy helps ensure that funding, support, and strategic initiatives are distributed more equitably. Ultimately, this balanced approach can foster innovation and drive progress in areas that might otherwise be overlooked, leading to a more inclusive and socially beneficial advancement of science.

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A Additional Related Work

We include additional related work here because of the space limitation in the main text.
Clustering with LLMs: Recent advances in clustering methodologies augmented by LLMs have demonstrated effective ways to generate interpretable groupings of text. For example, (Viswanathan et al., 2024; Katz et al., 2024) apply few-shot clustering and thematic grouping to partition scientific literature into meaningful subtopics, while (Zhang et al., 2023; Wang et al., 2023) further refine these techniques by aligning clustering outcomes with natural language explanations and user intent. Other recent work iteratively refines cluster representations by replacing cluster centroids or summary points with LLM-generated natural language descriptions and inclusion criteria, thereby inducing more abstract, interpretable concepts over multiple clustering rounds (Lam et al., 2024; Diaz-Rodriguez, 2025). While these approaches improve clustering quality by using LLMs at various stages, they mostly result in flat groupings rather than hierarchical structures. Our approach builds on this by using LLMs to cluster documents and organizing these clusters into a structured hierarchy.

Structured knowledge in LLMs: Prior work has explored how LLMs internalize hierarchical knowledge. For example, (He et al., 2024; Lovón-Melgarejo et al., 2023; Park et al., 2025) extend the linear representation hypothesis to reveal that LLMs encode categorical concepts as polytopes, with hierarchical relationships reflected as orthogonal directions. Other works such as (Wolfman et al., 2024) and (Budagam et al., 2024) examine the benefits of explicit hierarchical syntactic structures and prompting frameworks for guiding LLM performance, while (Moskvoretskii et al., 2024) and (Hu et al., 2024a) focus on constructing and materializing large-scale structured knowledge bases about entities and events. In line with the same aspirations, our work explores the use of hierarchical structures to organize scientific literature.

Structured knowledge representation: Understanding and organizing knowledge is a fundamental pursuit in both artificial and human intelligence (Dahlberg, 1993). Abstraction hierarchies, such as WordNet for lexical semantics (Miller, 1995), ConceptNet for commonsense reasoning (Speer et al., 2017), and Probase for large-scale concept representation (Wu et al., 2012), have proven to be powerful tools for structuring information. Similarly, modern tabular reasoning leverages structured representations to facilitate systematic inference and knowledge retrieval, demonstrating that such structure remains crucial (Wang et al., 2024).

B Evaluation Framework

We provide more context on our evaluation. As discussed in §5.2, we use randomly-sampled papers (title/abstract) as a query. The evaluator LLM goes through the hierarchy, starting from the root node and iteratively selects the relevant nodes to traverse. The prompt for each decision is shown in Fig.2.

Evaluation Framework

You are a scientist expert in taxonomy. Please read the following paper title and abstract.

Your task is to choose the next cluster/topic (while considering the current path) in the taxonomy that has the best chance of containing this paper.

Paper Title: {paper_title}
Paper Abstract: {paper_content}
Current Path: {path_so_far}

Choose from this cluster/topic list (MUST pick one):
{cluster_descriptions}

Required Response Format:
Cluster ID: [EXACT ID from the list] or Topic: [EXACT Category Name from the list]

Figure 2: Prompt used for Evaluation

One question is, **which LLM should we use for evaluation?** We chose `Qwen2.5-32b-instruct` for its strong instruction-following capabilities. In pilot experiments, Qwen showed a high consistency against GPT4 score, compared to other open-weight models. Here's a summary of that experiment: We evaluated one of the hierarchies produced by SCYCHIC using different models, including GPT-4. Assuming GPT-4 has the highest accuracy, we sought alternative models with the greatest consistency against it, as frequent evaluations with GPT4 are costly. Fig.5 presents the results. As it can be observed, Llama has the highest agreement, but we suspect bias since the hierarchy was also constructed with Llama. To avoid this, we selected the next best model, Qwen2.5-32b-instruct, for evaluation.

Evaluator LLLM	Agreement with GPT4
GPT-3.5	39.6
GPT4-mini	59.2
Gemma3-24b-it	62.1
Qwen2.5-32b-instruct	66.5
Llama 3.3 70B	72.4

Table 5: Agreement of different evaluator LLMs against GPT4.

C Extracting Paper Contributions

Below are prompts and examples for extracting different contributions (*problem*, *solution*, *result* and *topics*) from papers' titles and abstracts. we utilize the GPT-4o model (`gpt-4o-2024-08-06`) to generate all contribution extractions along with detailed rationales explaining the extraction decisions.

C.1 Prompt for Extracting *Problem/Solution/Result* Contributions

We use the prompt below to extract contributions from the paper's title and abstract. After finishing the extraction, the three contributions will be saved into the original `json` file. Please see §3.2 for more information.

Contributions Extraction from Paper

Consider the following following paper:

Title: {title}

Abstract: {abstract}

Extract the relevant content of the above abstract into the following JSON structure.
For certain fields that the information is not found in the abstract, leave them empty (empty string).

```
{
        "problem": {
                "overarching problem domain": "".
                "challenges/difficulties": "",
                "research question/goal": "",
                "novelty of the problem": "",
                "knowns or prior work": "",
        },
        "solution": {
                "overarching solution domain": "".
                "solution approach": "",
                "novelty of the solution": "",
                "knowns or prior work": "",
        },
        "results": {
                "findings/results": "",
                "potential impact of the results": "",
        }
}
```

Figure 3: Prompt for extracting *Problem/Solution/Result* contributions

C.2 Prompt for Extracting *Topic* Contributions and Rationales

This section has the prompt of generating topics and rationales from papers given their titles and abstracts. The prompt provides the model with a system role instruction that describes the task, title, and abstract, and also an example to get the specified output format.

Topics and Rationales Generation

~~~
You are an experienced scientist who is going to read and review research papers.

Paper Title: {title}
Paper Abstract: {abstract}

Read the above given Title and Abstract for a research paper and
Generate topics that are represented in the given Title and Abstract.
Example output format:
```json
{
 "topics": [
  {
   "topic": "Entity Taxonomy Creation",
   "rationale": "The research focuses on generating a comprehensive entity taxonomy using
LLMs."
  },
  {
   "topic": "Iterative Prompting Techniques",
   "rationale": "Highlights the use of iterative prompting to refine entity classifications."
  },
  {
   "topic": "GPT-4 and GPT-4 Turbo",
   "rationale": "Explores the capabilities of these advanced LLMs in taxonomy development."
  },
  {
   "topic": "Information Extraction",
   "rationale": "Demonstrates applications like relation and event argument extraction."
  },
  {
   "topic": "Computational Linguistics",
   "rationale": "Emphasizes contributions to AI-related and linguistic computational tasks."
  }
 ]
}
```
~~~

Figure 4: Prompt of *Topic* and *Rationale* Generation

C.3 Examples for *Problem/Solution/Result/Topic* contributions extracted from papers

Below we show examples of paper titles and abstracts, and different contributions (*Problem/Solution/Result/Topic*) we extract by language model.

Problem/Solution/Result/Topic *contributions from scientific papers*

Title: Sixfold excitations in electrides

Abstract: Due to the lack of full rotational symmetry in condensed matter physics, solids exhibit new excitations beyond Dirac and Weyl fermions, of which the sixfold excitations have attracted considerable interest owing to the presence of maximum degeneracy in bosonic systems. Here, we propose that a single linear dispersive sixfold excitation can be found in the electride Li$_{12}$ Mg$_3$ Si$_4$ and its derivatives. The sixfold excitation is formed by the floating bands of elementary band representation A@12a originating from the excess electrons centered at the vacancies (i.e., the 12a Wyckoff sites). There exists a unique topological bulk-surface-edge correspondence for the spinless sixfold excitation, resulting in trivial surface "Fermi arcs" but topological hinge arcs. All gapped k$_z$ slices belong to a two-dimensional higher-order topological insulating phase, which is protected by a combined symmetry T S$_{4z}$ and characterized by a quantized fractional corner charge Q$_{corner}$ = 3|e|/4. Consequently, the hinge arcs are obtained in the hinge spectra of the S$_{4z}$-symmetric rod structure. The state with a single sixfold excitation, stabilized by both nonsymmorphic crystalline symmetries and time-reversal symmetry, is located at the phase boundary and can be driven into various topologically distinct phases by explicit breaking of symmetries, making these electrides promising platforms for the systematic studies of different topological phases.

Contribution - Problem Statement

```
{
 "overarching_problem_domain":
    "Condensed matter physics",
 "challenges/difficulties":
    "Lack of full rotational symmetry
    in solids leading to new excitatio
    beyond Dirac and Weyl fermions",
 "research_question/goal":
    "Investigate sixfold excitations
    in electrides"
}
```

Contribution - Solution Statement

```
{
 "overarching_solution_domain":
    "Electrides and topological phases
 "solution_approach":
    "Propose that a single linear
    dispersive sixfold excitation can
    be found in the electride
    Li$_{12}$Mg$_3$Si$_4$ and its derivatives",
 "novelty_of_the_solution":
    "Unique topological bulk-surface-e
    correspondence for the spinless
    sixfold excitation"
}
```

Contribution - Result Statement

```
{
 "findings/results":
    "The sixfold excitation is formed by
    floating bands of elementary band
    representation A@12a. All gapped
    k$_z$ slices belong to two-dimensional
    higher-order topological insulating
    phase, characterized by a quantized
    fractional corner charge Q$_{corner}$ = 3|e|/4.
    Hinge arcs are obtained in the hinge
    spectra of the S$_{4z}$-symmetric rod
    structure.",
 "potential_impact_of_the_results":
    "Electrides are promising platforms
    for systematic studies of different
    topological phases."
}
```

Contribution - Topic: *'Electrides', 'Electrides in Condensed Matter Physics', 'Higher-Order Topological Insulators', 'Non-symmorphic Symmetries', 'Sixfold Excitation in Solids', 'Sixfold Excitations', 'Symmetry Breaking in Topological Materials', 'Topological Bulk-Surface-Edge Correspondence', 'Topological Phase Transitions', 'Topological Phases in Condensed Matter Physics', 'Topological Properties'*

Title: The Tin Pest Problem as a Test of Density Functionals Using High-Throughput Calculations

Abstract: At ambient pressure tin transforms from its ground-state semi-metal α-Sn (diamond structure) phase to the compact metallic β-Sn phase at 13 $\bullet$ C (286K). There may be a further transition to the simple hexagonal γ-Sn above 450K. These relatively low transition temperatures are due to the small energy differences between the structures, $\approx$ 20 meV/atom between α-and β-Sn. This makes tin an exceptionally sensitive test of the accuracy of density functionals and computational methods. Here we use the high-throughput Automatic-FLOW (AFLOW) method to study the energetics of tin in multiple structures using a variety of density functionals. We look at the successes and deficiencies of each functional. As no functional is completely satisfactory, we look Hubbard U corrections and show that the Coulomb interaction can be chosen to predict the correct phase transition temperature. We also discuss the necessity of testing high-throughput calculations for convergence for systems with small energy differences.

Contribution - Problem Statement

```
{
 "overarching_problem_domain":
    "Density functionals and computati
    methods for phase transitions in
    materials.",
 "challenges/difficulties":
    "Small energy differences between
    phases of tin make it a sensitive
    test for the accuracy of density
    functionals.",
 "research_question/goal":
    "To study the energetics of tin in
    multiple structures using a variet
    of density functionals and assess
    their accuracy."
}
```

Contribution - Solution Statement

```
{
 "overarching_solution_domain":
    "High-throughput computational
    methods and density functional
    theory.",
 "solution_approach":
    "Using the high-throughput
    Automatic-FLOW (AFLOW) method
    to study tin's energetics with
    various density functionals.",
 "novelty_of_the_solution":
    "Application of Hubbard U
    corrections to improve predictions
    of phase transition temperatures."
}
```

Contribution - Result Statement

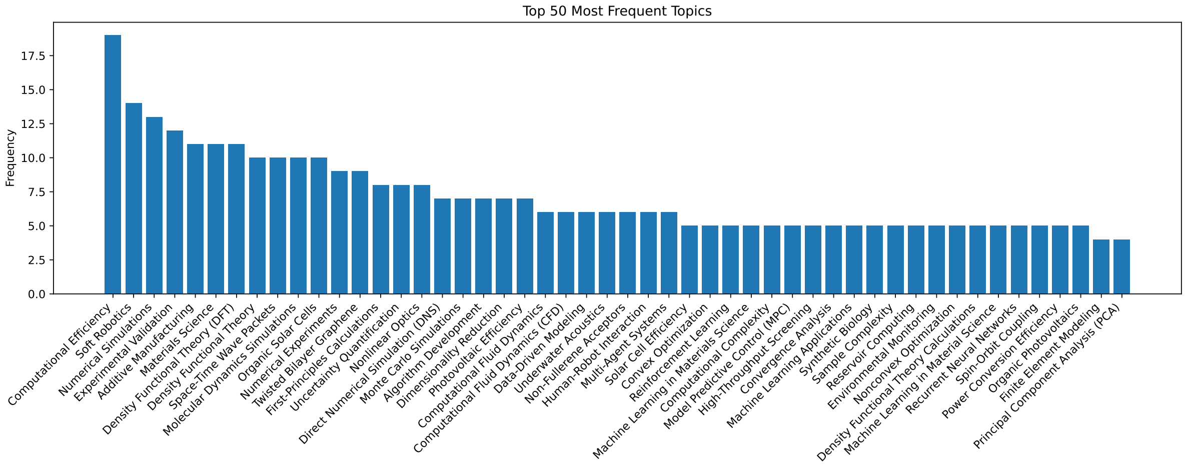
```
{
 "findings/results":
    "No functional is all satisfactory,
    but Hubbard U corrections can be chosen
    to predict the correct phase
    transition temperature.",
 "potential_impact_of_the_results":
    "Improved accuracy in predicting
    phase transitions in materials
    with small energy differences."
}
```

Contribution - Topic: *'Convergence Testing in Computational Simulations', 'Density Functional Theory (DFT) Accuracy', 'High-Throughput Computational Methods', 'Hubbard U Corrections', 'Tin Phase Transitions'*

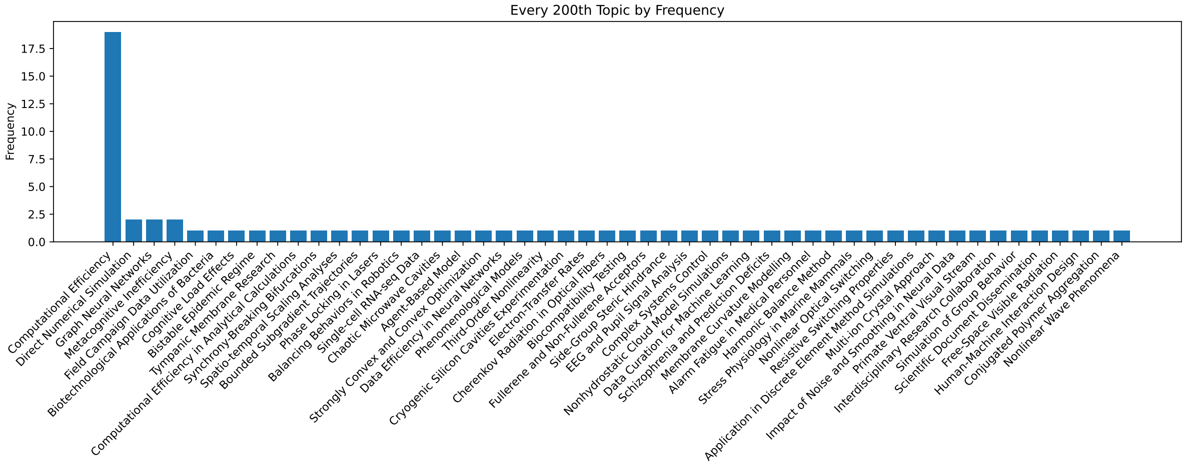
Table 6: Examples of extracted *problem/solution/result/topic* contributions from scientific paper abstracts.

C.4 Distribution of Extracted Topics

This section shows the distribution of various topics extracted from the papers based on frequency. This gives us an idea of what kind of topics were extracted.



(a) Top-50 topics by frequency in decreasing order



(b) Sampled topics (every 200)

Figure 5: Distribution of topics extracted from **SciPile**: (a) Top-50 topics, (b) Every 200 topics. Refer §3.2 for more information.

D Compiling a Seed Hierarchy

As we discuss in §4.3, we make a few adjustments to the seed hierarchy that we obtain from Wikipedia. Specifically:

1. We added “Theoretical Computer Science” and “Information Theory” as separate branches under “Formal Sciences” due to their unique characteristics;
2. We moved “Astronomy” under “Physical Science”;
3. “Astronomy”, “Geology” and “Oceanography” are listed under “Earth Science” but since these topics are not specific to early, we move them up one layer so that they’re directly under “Physical Science”; The Wikipedia article groups Geology, Oceanography, and Meteorology under ;
4. We added “History” as a branch under “Social Sciences”;
5. We included “Cell Biology” and “Genetics” under “Biological Sciences” as they were relevant and their inclusion would only help in better hierarchy creation.

These modifications aim to refine the hierarchy, ensuring it accurately reflects the distinct areas within each scientific domain. The resulting hierarchy is included in Fig.6.

```
{
    "Science":{
        "Formal Sciences":{
            "Logic":{},
            "Mathematics":{},
            "Statistics":{},
            "Computer Science":{},
            "Information Theory":{},
            "Systems Theory":{},
            "Decision Theory":{}
        },
        "Natural Sciences":{
            "Physical Science":{
                "Physics":{
                    "Classical Mechanics":{},
                    "Thermodynamics and statistical mechanics":{},
                    "Electromagnetism and photonics":{},
                    "Relativity":{},
                    "Quantum Mechanics":{},
                    "Atomic and molecular physics":{},
                    "Condensed matter physics":{},
                    "Optics and acoustics":{},
                    "High energy particle physics":{},
                    "Nuclear physics":{},
                    "Cosmology":{},
                    "Interdisciplinary Physics":{}
                },
                "Chemistry":{
                    "Physical Chemistry":{},
                    "Organic Chemistry":{},
                    "Inorganic Chemistry":{},
                    "Analytical Chemistry":{},
                    "Biological Chemistry":{},
                    "Theoretical Chemistry":{},
                    "Interdisciplinary Chemistry":{}
                },
                "Earth Science":{},
                "Astronomy":{},
                "Geology":{},
                "Oceanography":{},
                "Meteorology":{}
            },
            "Biological Sciences":{
                "Biochemistry":{},
                "Cell Biology":{},
                "Genetics":{},
                "Ecology":{},
                "Microbiology":{},
                "Botany":{},
                "Zoology":{}
            }
        },
        "Social Sciences":{
            "Anthropology":{},
            "Economics":{},
            "Political Science":{},
            "Sociology":{},
            "Psychology":{},
            "Geography":{},
            "History":{}
        }
    }
}
```

Figure 6: The seed hierarchy used by our FLMSci baselines. See §D for details.

E FLMSci: LLM-based Baselines

This section includes the pipeline and prompts used for FLMSci (parallel) and FLMSci(incremental).

E.1 Pipeline for FLMSci (parallel)

This section demonstrates the pipeline used for FLMSci (par) right from extracting topics and rationales to obtaining a final taxonomy with papers. (Refer to §4.3 for more information).

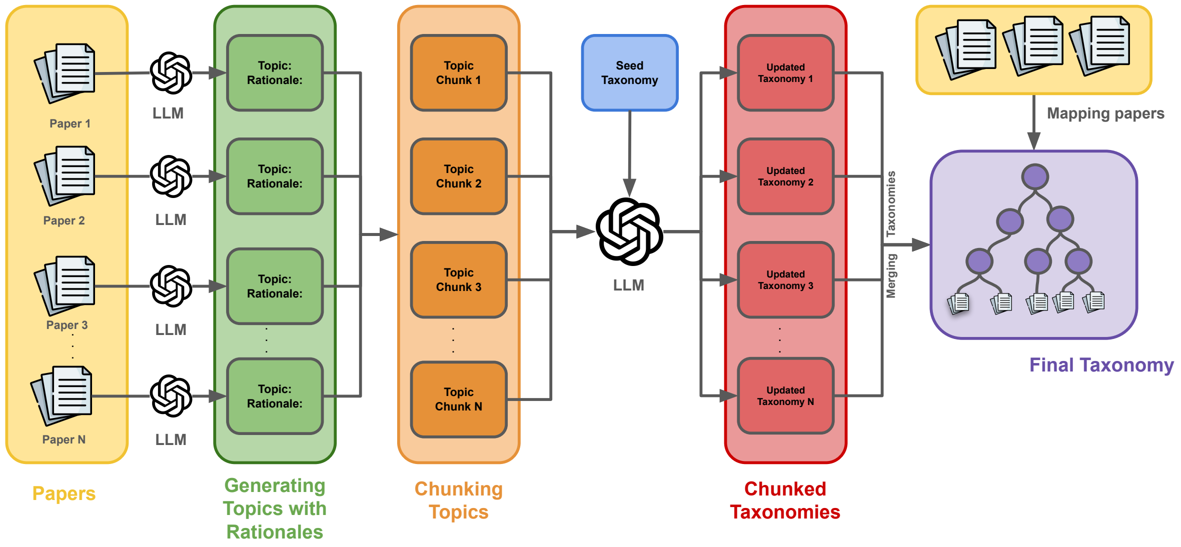


Figure 7: Pipeline for of FLMSci (parallel).

E.2 Prompt for fLMSci (parallel)

This prompt guides a large language model (LLM) to expand an existing scientific taxonomy - the seed taxonomy (Refer to D) by adding a set of new topics in a logical and consistent manner. With a clear list of instructions it ensures accurate placement and also preserves the original structure. This prompt was used with `Llama-3.3-70B-Instruct`. (Refer to §4.3 for more information.)

fLMSci (parallel) Prompt

You are a scientific domain expert. You have an initial "seed taxonomy" of scientific concepts and a list of new topics to integrate into that taxonomy. Please carefully analyze these new topics and update the seed taxonomy so that:

1. You must retain the current structure of the seed taxonomy and respect all existing categories.

2. Place each and every topic from the list given below.

2. You are free to add new branches or subcategories only where necessary to fit the new topics in a consistent, hierarchical ("is-a") manner.

3. Each topic from the list must appear exactly once. Do not introduce any new topics beyond those in the list.

4. Ensure each new topic is placed under the correct parent concept based on its semantic meaning or specialization level.

5. Return your updated taxonomy as valid JSON, containing both the original seed hierarchy and the newly incorporated topics.

Below is your seed taxonomy (in JSON). Make sure to preserve its structure as much as possible:

{seed_taxonomy}

Here is the list of new topics that must be integrated:

{topics_chunk}

Focus on logical placement of each term to maintain an accurate scientific hierarchy.

Figure 8: Prompt of fLMSci (incremental) pipeline

E.3 Demonstration of actions for FLMSci (incremental)

This section demonstrates the various actions (`add sibling`, `make parent`, `go down` and `discard`) that are available for the LLM to take at various levels of taxonomy building. Refer to §4.3 for more information.

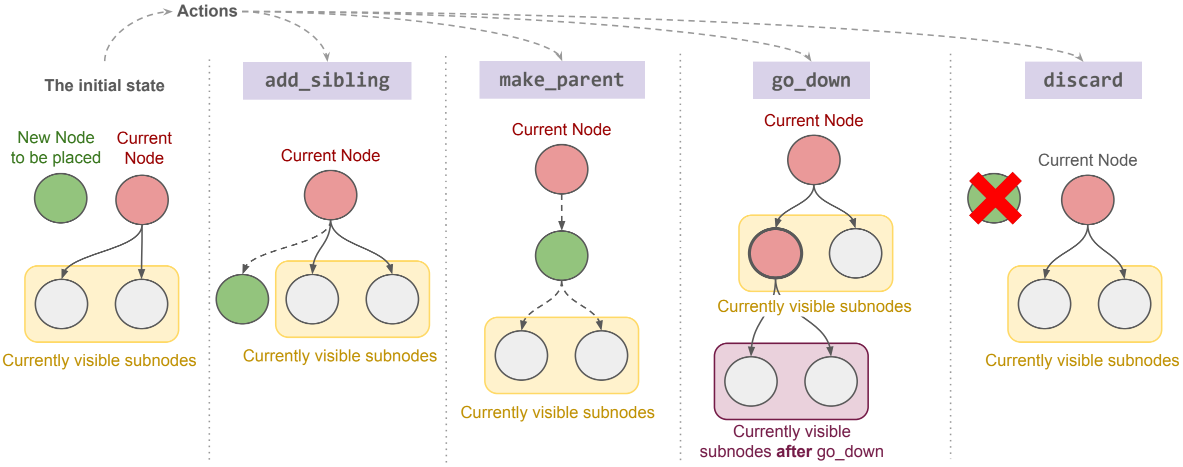

Actions
The initial state
New Node to be placed
Current Node
Currently visible subnodes
add_sibling
Current Node
Currently visible subnodes
make_parent
Current Node
Currently visible subnodes
go_down
Current Node
Currently visible subnodes
Currently visible subnodes after go_down
discard
Current Node
Currently visible subnodes

Figure 9: Actions for FLMSci (incremental)

E.4 Prompt for FLMSci (incremental)

This prompt is used to place new scientific topics into an existing seed taxonomy (Refer §D) incrementally. The model evaluates multiple possible actions based on the available action options. The prompt clearly instructs its priorities explicitly to give a hint to the model. The example usage and example output format help to get the response in a valid format. This prompt was used for `Llama-3.3-70B-Instruct`.

```
SUBNODE_DESCRIPTIONS = {
  "Formal Sciences": "Focuses on abstract systems and formal methodologies grounded in logic,
     mathematics, and symbolic reasoning. Provides theoretical frameworks (e.g., statistics, computer
      science, systems theory) used to model and solve problems across empirical disciplines and
     technology.",
  "Natural Sciences": "Investigates the physical universe and living organisms through empirical
     observation, experimentation, and theoretical analysis. Includes physical sciences (e.g.,
     physics, chemistry, astronomy) and biological sciences (e.g., genetics, ecology) to uncover
     fundamental laws and processes governing nature.",
  "Social Sciences": "Studies human behavior, societies, and institutions using qualitative and
     quantitative methods. Encompasses disciplines like psychology, economics, and political science
     to analyze cultural, economic, and social interactions within historical and geographic contexts
     ."
}
```

Figure 10: Descriptive statement used for contextualizing layer-1 items in the seed hierarchy, used in FLMSci (incremental). See §4.3 for broader context.

```
You are building a scientific topics based hierarchy.

Path traced until now: {current_path}
Subnode options available at this level:
subnodes = [{subnodes}]
New topic: "{new_topic}"

Evaluate all possible actions listed below equally before choosing the most appropriate one.
Choose the action that best preserves a logical hierarchy, semantic clarity, and appropriate abstraction level.

**Priority Guidance**:
1. FIRST consider "go_down" if ANY existing subnode could reasonably contain the new topic as a specialization
2. THEN consider "make_parent" if multiple existing subnodes could be grouped under a new category
3. ONLY use "add_sibling" if the topic is FUNDAMENTALLY distinct from all existing subnodes at this level
4. "discard" should be used for low-quality or redundant topics

**Critical Rules**:
- A node about "Applications of X" should ALWAYS go under X, not as a sibling
- Specific methods/tools belong under their parent field (e.g., "PCR" under "Molecular Biology")
- Avoid creating flat structures

Possible actions:
1) "go_down" - Use this if the topic: {new_topic} is a *more specific* subtype of one of the "subnodes" and belongs *within* it.
2) "add_sibling" - Use this if the topic: {new_topic} is on the same level of abstraction as the existing "subnodes". It should be added *alongside* them as a direct child of `{current_path[-1]}`.
3) "discard" - Use this if the topic: {new_topic} is irrelevant, redundant, or already captured under another topic.
4) "make_parent" - Use this when the new topic: {new_topic} or any one of the "subnodes" is broader or more abstract than one or more of the subnodes. In that case, make the new topic a direct child of `{current_path[-1]}` and move the relevant subnodes under it. Return them in `"child_nodes": [...]`.

### Example of desired usage for each action:
1) "go_down"
   - "node": must be the name of one of the existing "subnodes"
   - "explanation": an optional text with reasoning
   - "child_nodes", "parent_node": not used.

2) "add_sibling"
   - "node": {new_topic}
   - "parent_node": {current_path[-1]}
   - "explanation": optional
   - "child_nodes": not used.

3) "discard"
   - "node": {new_topic}
   - "explanation": optional
   - "parent_node", "child_nodes": not used

4) "make_parent"
   - "node": {new_topic} or one of the "subnodes" whichever is more appropriate
   - "child_nodes": array of the subnodes that must be moved under the new node
   - "explanation": optional
   - "parent_node": not used

Your output must be valid JSON only:
{{
  "action": "go_down"|"add_sibling"|"make_parent"|"discard",
  "node": "string",
  "parent_node": "string or null",  // only used if action = add_sibling
  "child_nodes": ["string", ...],   // only used if action = make_parent
  "explanation": "string (optional)"
}}
No extra text.
```

Figure 11: The detailed prompt used in the execution of our FLMSCI (incremental) baseline. See §4.3 for broader context.

F Further Details on Collection of Science Papers

This section provides more context on our piles of papers in our experiments from §5.1. **SciPileLarge** is an extension of **SciPile**. For each paper in **SciPile**, we extract five relevant keywords using an LLM (see Fig.12) and query the Semantic Scholar API[3] with these keywords to retrieve additional relevant papers.

We apply three filtering criteria to ensure quality: (a) **Citation Count:** A paper must have a minimum number of citations to be considered reliable. The minimum citation count is calculated using the formula: $(2 + 3 \times (2025 - \texttt{publish\_year})$. (b) **Abstract Length:** A paper must have an abstract with at least 250 tokens, as measured by the tokenizer of `Llama-3.1-8B-Instruct`. (c) **Publication Venue:** A paper must be published in a recognized journal or conference. For each keyword, we select up to five papers that meet all criteria. This approach maintains the disciplinary distribution of our seed dataset **SciPile**while expanding our corpus to $10K$ papers.

Keyword Extraction for Dataset Expansion

Title: {title}

Abstract: {abstract}

Generate exactly 5 relevant keyword phrases for this research paper. Each keyword phrase should be no more than 6 words long.

Return only a JSON array containing these 5 keywords. No explanations or other text.

Figure 12: Prompt of Keyword Extraction for Dataset Expansion

G Hyperparameters of Scychic

Here shows the models and hyperparameters we use for the experiments mentioned in §5.3. We utilize the GPT-4o model (`gpt-4o-2024-08-06`) to generate all contribution extractions along with detailed rationales explaining the extraction decisions. For `summarizer`, we use We choose `Llama-3.3-70B-Instruct`(Grattafiori et al., 2024) for its superiority of following instructions among open-source models, and use `gte-Qwen2-7B-instruct` as our `embedder`. For clustering algorithm, we apply k-means clustering. The number of clusters for each layer is (6, 40, 276) when conducting experiments on **SciPile** ($2K$ papers), and (6, 40, 276, 1250) when on **SciPileLarge** ($10k$ papers).

[3] https://www.semanticscholar.org/product/api

H Additional Experiments of SCYCHIC

H.1 Detailed Evaluation Results on *Topic* Contributions

Here we show the complete evaluation results mentioned in §5.2. SCYCHIC, FLMSci (**par**allel) and FLMSci(**inc**remental) are using *Topic* as contribution type.

Method	Accuracy (%)		LLM Cost		Hierarchy Structure				
	Strict-Acc ↑	L1-Acc ↑	Avg. # of Input Tokens ↓	# of Calls ↓	Max Depth	Avg Depth	Avg Bran. Factor	Max Bran. Factor	# of Items
Contributions type: Topic									
SCYCHIC	**14.9** ± 2.7	**65.7** ± 4.4	5017	322	3	3	40.9	128	11k
↳Top-down	14.5 ± 4.7	62.5 ± 7.4	6440	322	3	3	40.9	104	11k
↳Bottom-up	13.9 ± 5.3	54.4 ± 12.7	3988	322	3	3	40.9	119	11k
↳FLMSci (par)	4.0 ± 2.8	32.0 ± 6.3	8896	226	9	6.2	13.9	734	**9.9K**
↳FLMSci (inc)	**18.0** ± 5.3	**91.0** ± 4.0	4040	**61K**	14	7.7	3.6	704	**10.4K**

Table 7: Evaluation results of SCYCHIC, FLMSci (**par**allel) and FLMSci(**inc**remental) when using *Topic* as contribution type. "Bran." stands for "Branching". All methods show poor Strict-Acc ($\leq$ 18.0%), highlighting the challenging nature of the task. On one hand, FLMSci (inc) achieves the highest accuracy, showing the feasibility of building hierarchies by pure LLM-based methods. However, it incurs substantial computational costs, about 200× higher than other methods. In contrast, SCYCHIC offers a balanced performance profile with competitive accuracy (14.9% Strict-Acc, 65.7% L1-Acc) while maintaining significantly lower computational requirements.

H.2 Comparison of Different Embedding models

For the `embedder` mentioned in §4.1. We evaluate three embedding models—Qwen's `gte-Qwen2-7B-instruct` (Li et al., 2023), OpenAI's `text-embedding-3-large`, and `text-embedding-ada-002`. The first two performe similarly, whereas `text-embedding-ada-002` produce markedly weaker results. Given the comparable overall performance between the two leading models, we selecte `gte-Qwen2-7B-instruct` for our main experiments due to its strong balanced performance across both metrics, superior Sctric-Acc results, and practical advantages as an open-weight model that offers greater accessibility and cost-effectiveness for reproducible research.

Models→	`text-embedding-3-large`		`gte-Qwen2-7B-instruct`		`text-embedding-ada-002`	
Metrics→	L1-Acc	Sctric-Acc	L1-Acc	Sctric-Acc	L1-Acc	Sctric-Acc
PROBLEM	**86.7** ± 4.6	46.7 ± 0.9	81.7 ± 2.6	**51.1** ± 3.8	76.0 ± 4.4	41.7 ± 5.2
SOLUTION	80.3 ± 3.4	36.7 ± 1.7	**82.3** ± 1.1	**48.8** ± 6.1	63.5 ± 2.0	31.0 ± 3.2
RESULTS	**84.7** ± 5.7	44.0 ± 0.8	76.4 ± 6.9	**46.4** ± 5.2	74.6 ± 3.4	41.0 ± 8.7

Table 8: Performance comparison across three embedding models and contribution types. `gte-Qwen2-7B-instruct` demonstrates superior Sctric-Acc performance across all categories, while `text-embedding-3-large` excels in L1-Acc for *problem* and *results*. `text-embedding-ada-002` shows consistently weaker performance across both metrics.

H.3 Experiments of Prompt Engineering

We investigate the effect of different prompts on the final quality of hierarchy. In the main text, for the `summarizer` mentioned in §4.1, we use the detailed version prompt which is carefully curated. For comparison, we also conduct the experiments with a much simpler prompt.

Detailed (Curated) Prompt	**Simple Prompt**

You are a scientific research expert specializing in identifying and analyzing research problems and challenges. Your task is to analyze a collection of research papers or research clusters and provide a focused analysis of the research problems they address. The input could be either a collection of individual papers or research cluster summaries. Based on the content, you need to:
1. Identify the core research problems and challenges being addressed
2. Determine the overarching problem domain that connects these research efforts
3. Analyze the specific difficulties, gaps, or limitations that motivate this research
4. Understand the research questions or goals that drive these investigations
5. Generate an appropriate cluster name that captures the essence of the problem space
6. Provide a comprehensive problem-focused analysis
Here is the content to analyze:
Remember to:
• Focus specifically on problems, challenges, and research gaps rather than solutions
• Be specific about the technical difficulties and limitations being addressed
• Identify both theoretical and practical challenges
• Consider interdisciplinary connections in problem formulation
• Maintain scientific accuracy and use precise terminology
• Generate only one JSON format output that must follow the structure exactly
Please format your response as a JSON object with the following structure:
`{`
`"Cluster Name": "A clear and specific title focusing on the problem domain (No less than 5 words)",`
`"Problem": {`
`"overarching problem domain": "The broad scientific domain where these problems exist",`
`"challenges/difficulties": "Specific technical, theoretical, or practical challenges that these papers address",`
`"research question/goal": "The fundamental research questions or objectives that motivate this work"`
`}`
`}`
	You are a scientific research expert specializing in identifying and analyzing research problems and challenges. Analyze the input %s and output one JSON object:
	`{`
	`"Cluster Name": "A clear and specific title (No less than 5 words)",`
	`"Problem": {`
	`"overarching problem domain": "",`
	`"challenges/difficulties": "",`
	`"research question/goal": ""`
	`}`
	`}`
	Instructions Extract key themes and concepts. Identify the common thread that links the items. Craft a clear, specific title ($\geq$ 5 words) for Cluster Name. Return only the JSON—nothing else.

Table 9: Comparison of Detailed (Curated) and Simple Prompts

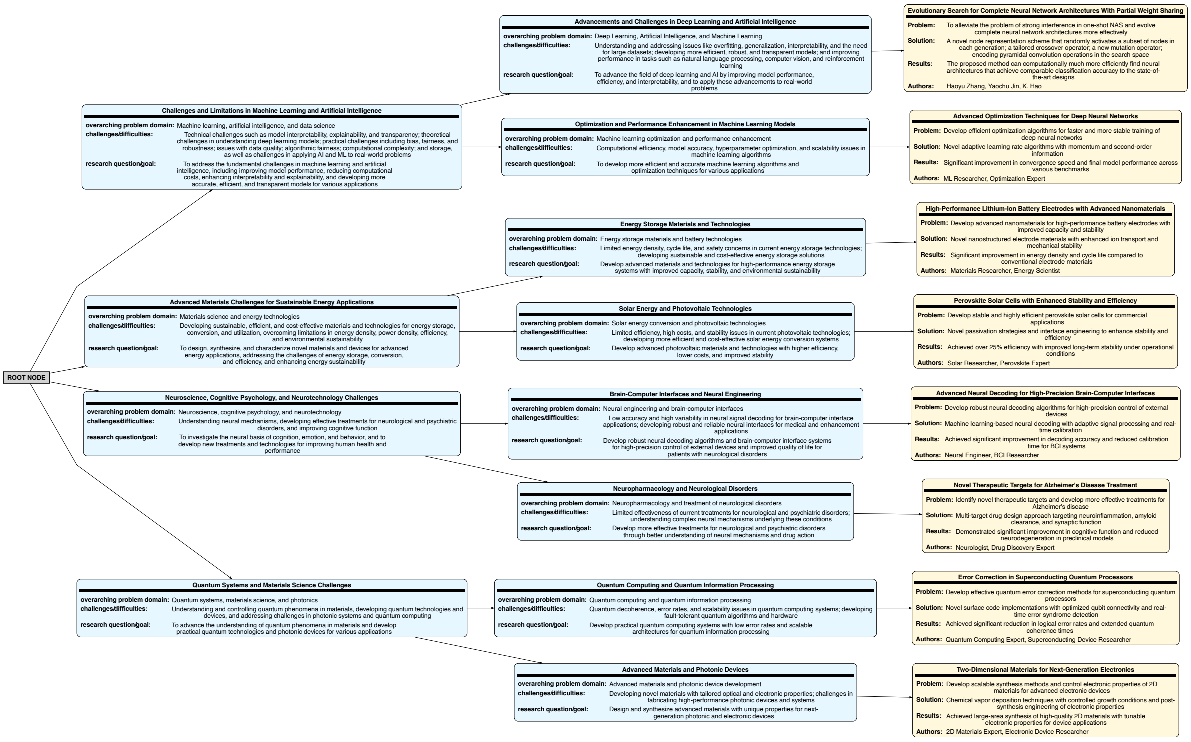
The results show that across all contributions, the curated prompt offers significantly better quality hierarchies.

Prompt type ↓	Embedder→	`text-embedding-3-large`		`gte-Qwen2-7B-instruct`	
	Metrics→	L1-Acc	Sctric-Acc	L1-Acc	Sctric-Acc
Simplified	*problem*	75.0 ± 4.6	33.7 ± 3.7	61.0 ± 0.8	24.7 ± 1.7
Detailed		**86.7** ± **4.6**	**46.7** ± **0.9**	**81.7** ± **2.6**	**51.1** ± **3.8**
Simplified	*solution*	65.3 ± 3.4	32.7 ± 2.6	59.0 ± 2.8	21.7 ± 2.9
Detailed		**80.3** ± **3.4**	**36.7** ± **1.7**	**82.3** ± **1.1**	**48.8** ± **6.1**
Simplified	*results*	77.7 ± 4.1	38.0 ± 4.6	66.7 ± 3.3	27.7 ± 2.5
Detailed		**84.7** ± **5.7**	**44.0** ± **0.8**	**76.4** ± **6.9**	**46.4** ± **5.2**

Table 10: Performance comparison between simplified and detailed prompts across different embedding models and contribution types. Detailed prompts consistently outperform simplified prompts across all scenarios, with improvements ranging from 7.0 to 23.3 % for L1-Acc and 3.0 to 26.4 % for Sctric-Acc. The `gte-Qwen2-7B-instruct` model shows the largest performance gains, with L1-Acc improvements of 20.7, 23.3, and 9.7 % for *problem*, *solution*, and *results* respectively.

I Demonstration of Hierarchy

Below is a snippet of our final hierarchy result.



Challenges and Limitations in Machine Learning and Artificial Intelligence
overarching problem domain: Machine learning, artificial intelligence, and data science
challenges/difficulties: Technical challenges such as model interpretability, explainability, and transparency; theoretical challenges in understanding deep learning models; practical challenges including bias, fairness, and robustness; issues with data quality; algorithmic fairness; computational complexity; and storage, as well as challenges in applying AI and ML to real-world problems
research question/goal: To address the fundamental challenges in machine learning and artificial intelligence, including improving model performance, reducing computational costs, enhancing interpretability and explainability, and developing more accurate, efficient, and transparent models for various applications

Advancements and Challenges in Deep Learning and Artificial Intelligence
overarching problem domain: Deep Learning, Artificial Intelligence, and Machine Learning
challenges/difficulties: Understanding and addressing issues like overfitting, generalization, interpretability, and the need for large datasets; developing more efficient, robust, and transparent models; and improving performance in tasks such as natural language processing, computer vision, and reinforcement learning
research question/goal: To advance the field of deep learning and AI by improving model performance, efficiency, and interpretability, and to apply these advancements to real-world problems

Evolutionary Search for Complete Neural Network Architectures With Partial Weight Sharing
Problem: To alleviate the problem of strong interference in one-shot NAS and evolve complete neural network architectures more effectively
Solution: A novel node representation scheme that randomly activates a subset of nodes in each generation; a tailored crossover operator; a new mutation operator; encoding pyramidal convolution operations in the search space
Results: The proposed method can computationally much more efficiently find neural architectures that achieve comparable classification accuracy to the state-of-the-art designs
Authors: Haoyu Zhang, Yaochu Jin, K. Hao

Optimization and Performance Enhancement in Machine Learning Models
overarching problem domain: Machine learning optimization and performance enhancement
challenges/difficulties: Computational efficiency, model accuracy, hyperparameter optimization, and scalability issues in machine learning algorithms
research question/goal: To develop more efficient and accurate machine learning algorithms and optimization techniques for various applications

Advanced Optimization Techniques for Deep Neural Networks
Problem: Develop efficient optimization algorithms for faster and more stable training of deep neural networks
Solution: Novel adaptive learning rate algorithms with momentum and second-order information
Results: Significant improvement in convergence speed and final model performance across various benchmarks
Authors: ML Researcher, Optimization Expert

Advanced Materials Challenges for Sustainable Energy Applications
overarching problem domain: Materials science and energy technologies
challenges/difficulties: Developing sustainable, efficient, and cost-effective materials and technologies for energy storage, conversion, and utilization, overcoming limitations in energy density, power density, efficiency, and environmental sustainability
research question/goal: To design, synthesize, and characterize novel materials and devices for advanced energy applications, addressing the challenges of energy storage, conversion, and efficiency, and enhancing energy sustainability

Energy Storage Materials and Technologies
overarching problem domain: Energy storage materials and battery technologies
challenges/difficulties: Limited energy density, cycle life, and safety concerns in current energy storage technologies; developing sustainable and cost-effective energy storage solutions
research question/goal: Develop advanced materials and technologies for high-performance energy storage systems with improved capacity, stability, and environmental sustainability

High-Performance Lithium-Ion Battery Electrodes with Advanced Nanomaterials
Problem: Develop advanced nanomaterials for high-performance battery electrodes with improved capacity and stability
Solution: Novel nanostructured electrode materials with enhanced ion transport and mechanical stability
Results: Significant improvement in energy density and cycle life compared to conventional electrode materials
Authors: Materials Researcher, Energy Scientist

Solar Energy and Photovoltaic Technologies
overarching problem domain: Solar energy conversion and photovoltaic technologies
challenges/difficulties: Limited efficiency, high costs, and stability issues in current photovoltaic technologies; developing more efficient and cost-effective solar energy conversion systems
research question/goal: Develop advanced photovoltaic materials and technologies with higher efficiency, lower costs, and improved stability

Perovskite Solar Cells with Enhanced Stability and Efficiency
Problem: Develop stable and highly efficient perovskite solar cells for commercial applications
Solution: Novel passivation strategies and interface engineering to enhance stability and efficiency
Results: Achieved over 25% efficiency with improved long-term stability under operational conditions
Authors: Solar Researcher, Perovskite Expert

Neuroscience, Cognitive Psychology, and Neurotechnology Challenges
overarching problem domain: Neuroscience, cognitive psychology, and neurotechnology
challenges/difficulties: Understanding neural mechanisms, developing effective treatments for neurological and psychiatric disorders, and improving cognitive function
research question/goal: To investigate the neural basis of cognition, emotion, and behavior, and to develop new treatments and technologies for improving human health and performance

Brain-Computer Interfaces and Neural Engineering
overarching problem domain: Neural engineering and brain-computer interfaces
challenges/difficulties: Low accuracy and high variability in neural signal decoding for brain-computer interface applications; developing robust and reliable neural interfaces for medical and enhancement applications
research question/goal: Develop robust neural decoding algorithms and brain-computer interface systems for high-precision control of external devices and improved quality of life for patients with neurological disorders

Advanced Neural Decoding for High-Precision Brain-Computer Interfaces
Problem: Develop robust neural decoding algorithms for high-precision control of external devices
Solution: Machine learning-based neural decoding with adaptive signal processing and real-time calibration
Results: Achieved significant improvement in decoding accuracy and reduced calibration time for BCI systems
Authors: Neural Engineer, BCI Researcher

Neuropharmacology and Neurological Disorders
overarching problem domain: Neuropharmacology and treatment of neurological disorders
challenges/difficulties: Limited effectiveness of current treatments for neurological and psychiatric disorders; understanding complex neural mechanisms underlying these conditions
research question/goal: Develop more effective treatments for neurological and psychiatric disorders through better understanding of neural mechanisms and drug action

Novel Therapeutic Targets for Alzheimer's Disease Treatment
Problem: Identify novel therapeutic targets and develop more effective treatments for Alzheimer's disease
Solution: Multi-target drug design approach targeting neuroinflammation, amyloid clearance, and synaptic function
Results: Demonstrated significant improvement in cognitive function and reduced neurodegeneration in preclinical models
Authors: Neurologist, Drug Discovery Expert

Quantum Systems and Materials Science Challenges
overarching problem domain: Quantum systems, materials science, and photonics
challenges/difficulties: Understanding and controlling quantum phenomena in materials, developing quantum technologies and devices, and addressing challenges in photonic systems and quantum computing
research question/goal: To advance the understanding of quantum phenomena in materials and develop practical quantum technologies and photonic devices for various applications

Quantum Computing and Quantum Information Processing
overarching problem domain: Quantum computing and quantum information processing
challenges/difficulties: Quantum decoherence, error rates, and scalability issues in quantum computing systems; developing fault-tolerant quantum algorithms and hardware
research question/goal: Develop practical quantum computing systems with low error rates and scalable architectures for quantum information processing

Error Correction in Superconducting Quantum Processors
Problem: Develop effective quantum error correction methods for superconducting quantum processors
Solution: Novel surface code implementations with optimized qubit connectivity and real-time error syndrome detection
Results: Achieved significant reduction in logical error rates and extended quantum coherence times
Authors: Quantum Computing Expert, Superconducting Device Researcher

Advanced Materials and Photonic Devices
overarching problem domain: Advanced materials and photonic device development
challenges/difficulties: Developing novel materials with tailored optical and electronic properties; challenges in fabricating high-performance photonic devices and systems
research question/goal: Design and synthesize advanced materials with unique properties for next-generation photonic and electronic devices

Two-Dimensional Materials for Next-Generation Electronics
Problem: Develop scalable synthesis methods and control electronic properties of 2D materials for advanced electronic devices
Solution: Chemical vapor deposition techniques with controlled growth conditions and post-synthesis engineering of electronic properties
Results: Achieved large-area synthesis of high-quality 2D materials with tunable electronic properties for device applications
Authors: 2D Materials Expert, Electronic Device Researcher

Figure 13: Above is a small example of a final hierarchy generated by SCYCHIC on the **SciPileLarge** dataset. The original hierarchy has 4 levels, use papers' *problem* contribution. Due to space constraints, this snippet shows only two levels of clusters above the individual papers.