METASCIENTIST: A Human-AI Synergistic Framework for Automated Mechanical Metamaterial Design

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Demo link: `http://zhoulab-1.cs.vt.edu:5557/`

Abstract

The discovery of novel mechanical metamaterials, whose properties are dominated by their engineered structures rather than chemical composition, is a knowledge-intensive and resource-demanding process. To accelerate the design of novel metamaterials, we present METASCIENTIST, a human-in-the-loop system that integrates advanced AI capabilities with expert oversight with two primary phases: (1) hypothesis generation, where the system performs complex reasoning to generate novel and scientifically sound hypotheses, supported with domain-specific foundation models and inductive biases retrieved from existing literature; (2) 3D structure synthesis, where a 3D structure is synthesized with a novel 3D diffusion model based on the textual hypothesis and refined it with a LLM-based refinement model to achieve better structure properties. At each phase, domain experts iteratively validate the system outputs, and provide feedback and supplementary materials to ensure the alignment of the outputs with scientific principles and human preferences. Through extensive evaluation from human scientists, METASCIENTIST is able to deliver novel and valid mechanical metamaterial designs that have the potential to be highly impactful in the metamaterial field[1].

1 Introduction

Metamaterials are microstructured materials whose properties go beyond those of the ingredient materials, often possessing unusual mechanical and/or functional properties (Kadic et al., 2019; Bertoldi et al., 2017; Jia et al., 2020; Jiao and Alavi, 2021; Bauer et al., 2017). The advancements in metamaterials have fostered a vast amount of technological innovations across various key domains, such as structural, sensing, actuation, and multifunctional materials innovations. However, human scientists are facing two critical challenges in designing and discovering novel metamaterials.

First, as the field of metamaterial expands exponentially, it becomes increasingly challenging for researchers to keep pace with the rapid accumulation of knowledge. For instance, the number of metamaterial-related publications has grown from 156 papers in 2000, 7,170 papers in 2010, to over 30,000 papers in 2023 based on Google Scholar statistics. The rapid proliferation of research has created significant barriers to effectively understanding and building upon existing work, ultimately slowing down the pace of technological innovation. Second, existing workflows for metamaterial design impose substantial cognitive and resource burdens throughout their multi-stage development process. From initial conceptualization through theoretical modeling, computational simulation, and experimental validation, each phase demands significant human expertise and creativity while incurring considerable time and financial costs. These combined constraints severely limit both the exploration of new concepts and the scaling of successful designs for practical applications.

Recent breakthroughs in large language models (LLMs) have inspired the development of *autonomous scientists* to automate aspects of the research process, such as generating novel research ideas and outlining implementation procedures (Zhang et al., 2024b). However, in specialized scientific domains like metamaterial design, several recent studies (Hong, 2023; Park et al., 2024; Deb et al., 2024) have highlighted significant limitations even in state-of-the-art models like GPT-4o (Hurst et al., 2024). While these models can *boldly* synthesize vast amounts of scientific knowledge and propose testable hypotheses, they are prone to high factual error rates, often stemming from confusion caused by similar nomen-

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[1] The demo video for METASCIENTIST is publicly available at: `https://drive.google.com/file/d/19HYCRYgEeuShJZgBUdSGI-18KD-cfBAp/view?usp=sharing`

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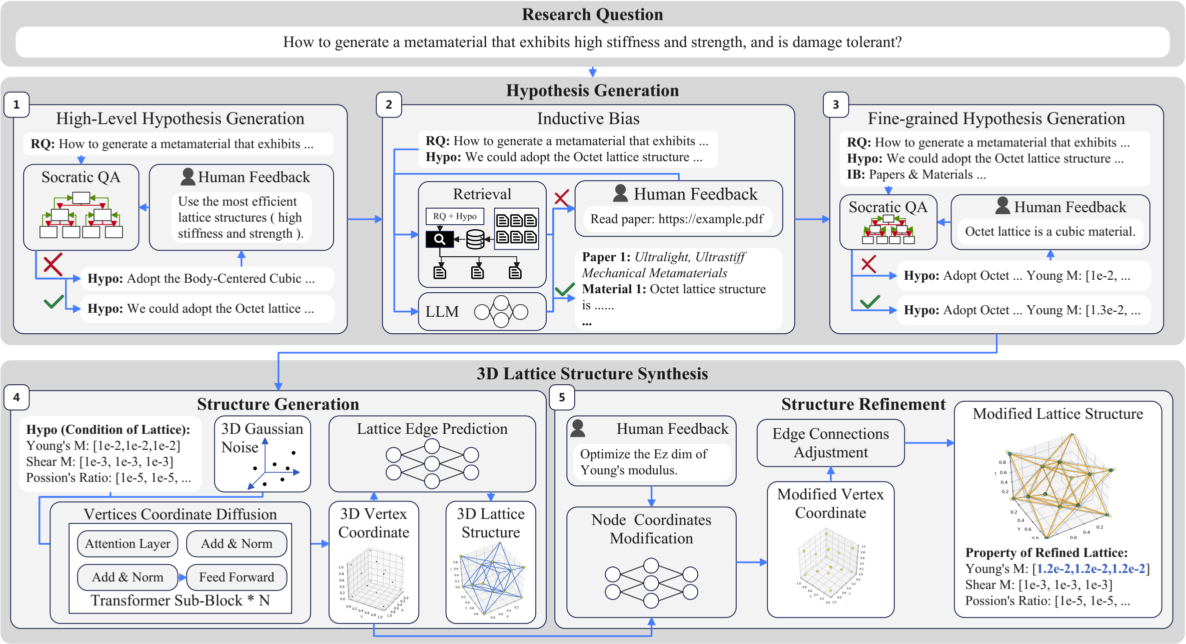

Figure 1: **Overview** of METASCIENTIST.

clatures across different fields or lack of rigorous logical reasoning and mathematical derivation capabilities, which are critical for scientific research. In addition, these models typically fail to assess the plausibility of their hypotheses effectively, and their proposals are often overly generic, offering limited practical value for real-world experiments.[2]

To tackle these challenges, we introduce METASCIENTIST, a human-in-the-loop system for assisting and accelerating novel metamaterial design, with a particular focus on mechanical metamaterials (e.g., lattice-based structures with superior mechanical properties). As depicted in Figure 1, METASCIENTIST comprises two key phases: **(1) Hypothesis Generation**: Given an input research question, we perform complex reasoning upon evidence and inductive biases retrieved from a large collection of materials science literature to generate novel hypotheses. **(2) 3D Structure Synthesis**: We build a 3D diffusion model to transform the generated textual hypotheses into 3D metamaterial structures, and then refine the generated structures with a LLM-based refinement model to achieve better structure properties (e.g., symmetry and periodicity)[3]. Throughout both phases, we involve human scientists to actively interact with our system and iteratively provide diverse types of feedback, including cutting-edge insights, error correction, and supplementary materials, to ensure the generated hypotheses are feasible, novel, and aligned with up-to-date domain knowledge in metamaterials. Our contributions are summarized as follows:

- We introduce METASCIENTIST, the first complete hypothesis generation system to facilitate novel metamaterial design by automating knowledge and resource-intensive procedures.
- METASCIENTIST involved domain experts in the loop to iteratively incorporate high-quality feedback from human scientists to ensure the validity and creativity of hypotheses.
- With extensive evaluation and case studies, we demonstrate METASCIENTIST has significant potential to advance AI-assisted metamaterial design and reduce the extensive cost and cognitive load required for human scientists.

2 Implementation of METASCIENTIST

2.1 Foundation Model for Metamaterials Science

While existing general-purpose LLMs excel at a wide range of NLP tasks, they often struggle in highly specialized domains such as materials science (Song et al., 2023). To address this challenge, we first collect 5,611 research papers and books

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[2] We provide examples in Appendix D to illustrate the key limitations of GPT-4o for automated metamaterial design.

[3] Though Metamaterials can have diverse types of structure morphologies, we mainly focus on lattice metamaterials as they are common and have a large design space.

from Google Scholar based on a list of keywords that are provided by a domain expert and related to metamaterial design or general domain knowledge of materials science. We then design a comprehensive data-cleaning process and convert them into plain text.[4] Based on this corpus, we finetune an open-sourced LLM, i.e., `Llama3-8B-Instruct`, using the Low-Rank Adaptation (LoRA) technique (Hu et al., 2022), and tailor the model to the metamaterials science domain. To qualitatively evaluate this model, we ask a domain expert to provide a list of question-answer pairs and compare it against an open-source LLM baseline.[5]

2.2 Hypothesis Generation

Generating novel, feasible, and scientifically sound hypotheses requires strong reasoning capability based on existing knowledge and literature. To this end, we equip our domain-specific foundation model in §2.1 with a recent state-of-the-art complex reasoning framework, i.e., Socratic Questioning (Qi et al., 2023), to generate novel hypotheses. Specifically, the hypothesis generation process consists of three key steps.

High-Level Hypothesis Generation Since the properties of lattice materials are dominated by their structure, in the first step, we focus on generating a high-level hypothesis that is novel and reasonable with normalized materials properties. With the Socratic Questioning module, we first perform a **top-down exploration** process that recursively decomposes a complex research question, e.g., *"how to generate a metamaterial that exhibits high stiffness and strength, and is damage tolerant"*, into several simpler sub-questions, such as *"what properties should a material have to be damage tolerant"*, and *"what are the common techniques to enhance both stiffness and strength"*. With the solutions of the sub-questions proposed by LLM itself, e.g., *"a material should have high Young's modulus and Shear modulus to be damage tolerant"*, we employ a **bottom-up backtracking** process selectively leverage these answers to infer the hypothesis to solve the original research question, e.g., *"Octet or Kelvin structures might be promising to solve the question"*.

While the Socratic Questioning module can generate seemingly reasonable hypotheses, our preliminary experiments show that these automatically generated high-level hypotheses still suffer from several critical issues, including hallucinations, limited novelty, or deviating from desired directions. Therefore, we involve domain experts to provide feedback, either natural language feedback or relevant papers, which are then incorporated as additional context when solving the original research question during the bottom-up backtracking process, encouraging the model to generate more valid and novel hypotheses that are aligned with human expectations.

Inductive Bias Extraction The hypotheses proposed by human scientists are inherently shaped by inductive biases, i.e., existing knowledge and initial assumptions. A valid and novel hypothesis needs to excel in two aspects: it must be grounded in established knowledge while offering distinct contributions beyond existing literature. Thus, we propose an inductive bias extraction module that extracts relevant knowledge from multiple sources, including (1) *internal inductive bias* which is elicited from LLM itself by prompting it based on an expert-written taxonomy[6], e.g., *Based on the taxonomy, compile a list of known lattice structures relevant to the hypothesis...*; and (2) *external inductive biases*, which are summaries of relevant articles retrieved from our collected literature corpus introduced in §2.1. In this process, we use the concatenation of an original research question and a high-level hypothesis as the query, `ColBERT` (Khattab and Zaharia, 2020) as the text encoder, and L2 as the distance metric to retrieve top-K relevant articles to the query. We then use GPT-4o to locate the relevant content to the query within each paper and summarize it into one paragraph for each article.

The inductive biases may contain information that is outdated or irrelevant to the query, thus we involve domain experts to either directly refine the outputs by removing undesired inductive biases or provide feedback to improve the retrieval process, such as providing additional keywords for more accurate retrieval, directly uploading relevant papers, or providing textual supplementary materials.

Fine-grained Hypothesis Generation We further leverage the inductive biases as additional evidence, i.e., feeding them together with the original research question as input to the Socratic Questioning module, to refine the initial hypothesis into a

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[4] We include more details for data collection and statistics in Appendix A.1.1

[5] Additional training and evaluation details for our domain-specific foundation model are provided in Appendix A.1.2.

[6] More details are provided in Appendix A.2

fine-grained description of features and attributes that inform the structure design of the new target metamaterial. In our system, we primarily consider three critical attributes, i.e., *Young's Modulus*, *Shear Modulus*, and *Poisson's Ratio*, for later 3D structure generation. As the model may not be able to capture all necessary lattice structure properties or the predicted attributes are not aligned with human experts' expectations, we allow human experts to enrich the dimensions of proposed lattice structure properties and adjust fine-grained details to meet specific requirements. We present a complete and concrete case study in §3 to demonstrate how our METASCIENTIST system generates a fine-grained hypothesis step-by-step.

2.3 3D Structure Synthesis

Our next step is to generate a 3D lattice structure that aligns with the previously generated hypothesis. This phase consists of two steps: generating 3D structures conditioned on the lattice properties in the fine-grained hypothesis using a diffusion model, and further refining the generated structures based on human feedback with a refinement model.[7]

3D Structure Generation As shown in Figure 2, the initial 3D structure is generated with two components: (1) **Vertices Coordinate Diffusion**, which generates the 3D coordinates of the lattice vertices. It takes two inputs: random Gaussian noise and the lattice properties derived from the hypothesis generated in the preceding phase. The Gaussian noise, which matches the dimensionality of the 3D vertex coordinates, is input as a sequence of 3-dimensional tuples. The lattice properties are incorporated into the diffusion model via an attention mechanism implemented in the transformer sub-blocks. Specifically, the attention mechanism uses three components: query, key, and value. The query term is generated through a linear projection of the lattice properties, while the key and value terms are derived either from the input Gaussian noise or from the output of the previous transformer sub-block. Through iterative denoising, the diffusion block progressively refines the 3D coordinates, transforming the initial noise into structured vertex positions that align with the given lattice properties. (2) **Lattice Edge Prediction**, which predicts edges between vertices. It uses a multi-layer perceptron (MLP) to evaluate the similarity between vertex representations and determine the presence or absence of edges. This module ensures the generated 3D lattice structure is cohesive and consistent with the hypothesized properties.

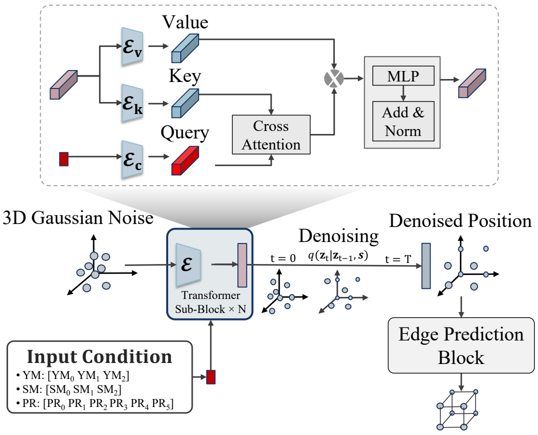

Figure 2: Illustration of 3D structure generation.

3D Structure Refinement While the 3D lattice generation module can produce new and reasonable structures, it's still challenging to ensure the symmetric structure or periodic boundary conditions, which are crucial for improving mechanical properties of the metamaterial. Therefore, we introduce a LLM-based structure refinement module. Inspired by Gruver et al. (2024), we feed the structure information as text into an LLM and refine the lattice structure in two sequential stages: (1) **Node Refinement**, where the model optimizes nodes' symmetry and periodicity by adjusting node positions, adding necessary nodes, and removing redundant ones; and (2) **Edge Refinement**, where the model adjusts edge connections on the new node layout so that the overall structures satisfy the periodic boundary conditions necessary for fabrication. Such a process is iterated for multiple cycles until the desired structure symmetry and periodicity are achieved simultaneously. Finally, once our model outputs the coordinates of each node and the edges between the nodes, we visualize the structure by plotting the nodes as a 3D scatter plot and the edges as 3D line segments via `matplotlib.pyplot` package.

3 Experiments and Evaluation

Case Study To demonstrate the effectiveness of METASCIENTIST, we present a case study focusing on a classical weight minimization problem in materials science, as shown in Figure 3. The weight minimization problem represents an ideal test case for METASCIENTIST as it combines fundamental materials science challenges with clear industrial applications - designing structures that

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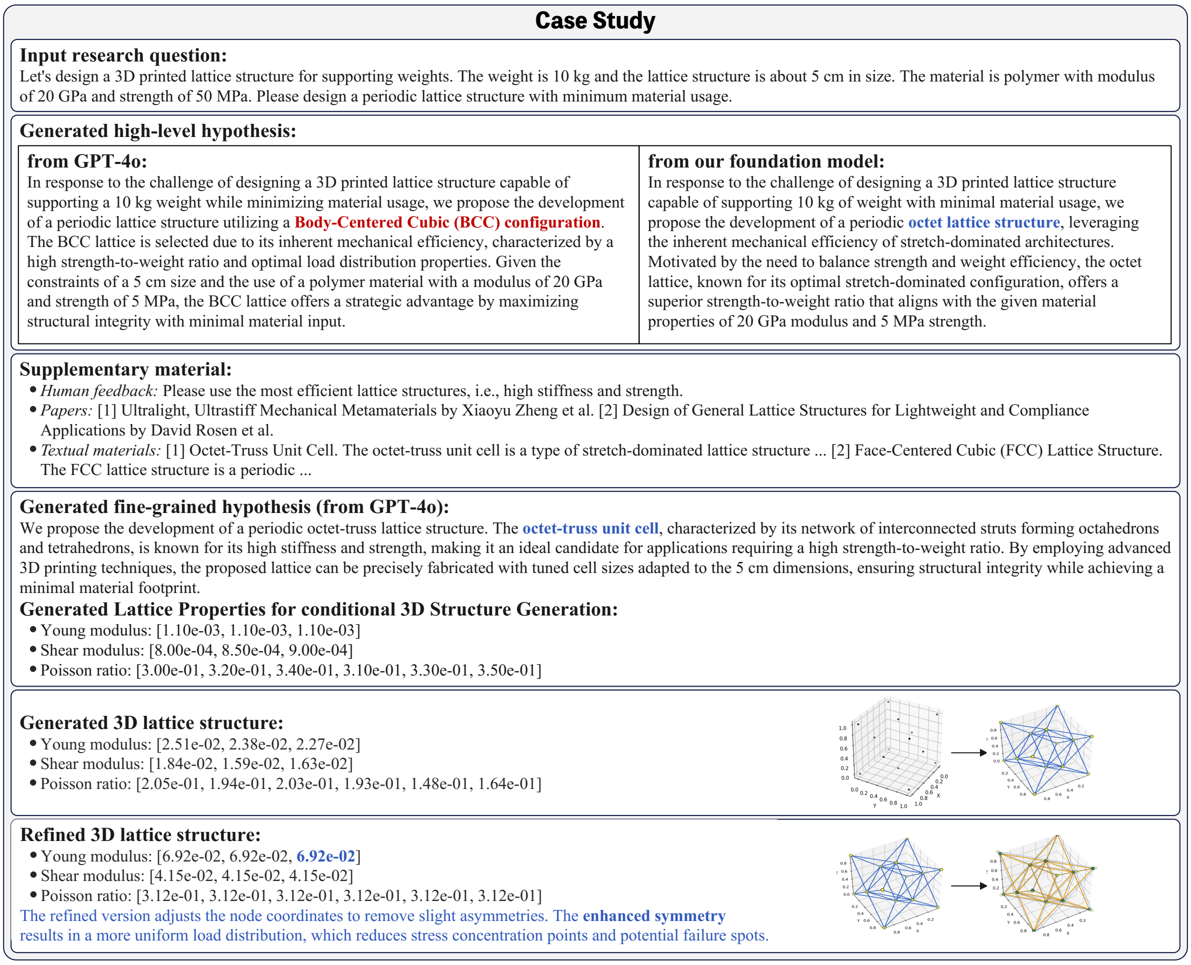
[7] Training details are provided in Appendix A.3.



Case Study

Input research question:
Let's design a 3D printed lattice structure for supporting weights. The weight is 10 kg and the lattice structure is about 5 cm in size. The material is polymer with modulus of 20 GPa and strength of 50 MPa. Please design a periodic lattice structure with minimum material usage.

Generated high-level hypothesis:

from GPT-4o:	**from our foundation model:**
In response to the challenge of designing a 3D printed lattice structure capable of supporting a 10 kg weight while minimizing material usage, we propose the development of a periodic lattice structure utilizing a **Body-Centered Cubic (BCC) configuration**. The BCC lattice is selected due to its inherent mechanical efficiency, characterized by a high strength-to-weight ratio and optimal load distribution properties. Given the constraints of a 5 cm size and the use of a polymer material with a modulus of 20 GPa and strength of 5 MPa, the BCC lattice offers a strategic advantage by maximizing structural integrity with minimal material input.	In response to the challenge of designing a 3D printed lattice structure capable of supporting 10 kg of weight with minimal material usage, we propose the development of a periodic **octet lattice structure**, leveraging the inherent mechanical efficiency of stretch-dominated architectures. Motivated by the need to balance strength and weight efficiency, the octet lattice, known for its optimal stretch-dominated configuration, offers a superior strength-to-weight ratio that aligns with the given material properties of 20 GPa modulus and 5 MPa strength.

Supplementary material:
- *Human feedback:* Please use the most efficient lattice structures, i.e., high stiffness and strength.
- *Papers:* [1] Ultralight, Ultrastiff Mechanical Metamaterials by Xiaoyu Zheng et al. [2] Design of General Lattice Structures for Lightweight and Compliance Applications by David Rosen et al.
- *Textual materials:* [1] Octet-Truss Unit Cell. The octet-truss unit cell is a type of stretch-dominated lattice structure ... [2] Face-Centered Cubic (FCC) Lattice Structure. The FCC lattice structure is a periodic ...

Generated fine-grained hypothesis (from GPT-4o):
We propose the development of a periodic octet-truss lattice structure. The **octet-truss unit cell**, characterized by its network of interconnected struts forming octahedrons and tetrahedrons, is known for its high stiffness and strength, making it an ideal candidate for applications requiring a high strength-to-weight ratio. By employing advanced 3D printing techniques, the proposed lattice can be precisely fabricated with tuned cell sizes adapted to the 5 cm dimensions, ensuring structural integrity while achieving a minimal material footprint.

Generated Lattice Properties for conditional 3D Structure Generation:
- Young modulus: [1.10e-03, 1.10e-03, 1.10e-03]
- Shear modulus: [8.00e-04, 8.50e-04, 9.00e-04]
- Poisson ratio: [3.00e-01, 3.20e-01, 3.40e-01, 3.10e-01, 3.30e-01, 3.50e-01]

Generated 3D lattice structure:
- Young modulus: [2.51e-02, 2.38e-02, 2.27e-02]
- Shear modulus: [1.84e-02, 1.59e-02, 1.63e-02]
- Poisson ratio: [2.05e-01, 1.94e-01, 2.03e-01, 1.93e-01, 1.48e-01, 1.64e-01]

Refined 3D lattice structure:
- Young modulus: [6.92e-02, 6.92e-02, **6.92e-02**]
- Shear modulus: [4.15e-02, 4.15e-02, 4.15e-02]
- Poisson ratio: [3.12e-01, 3.12e-01, 3.12e-01, 3.12e-01, 3.12e-01, 3.12e-01]

The refined version adjusts the node coordinates to remove slight asymmetries. The **enhanced symmetry** results in a more uniform load distribution, which reduces stress concentration points and potential failure spots.

Figure 3: **Case study** of using METASCIENTIST to solve the weight minimization problem.

maximize support while minimizing material usage requires sophisticated reasoning about mechanical constraints while allowing for quantitative evaluation through well-established metrics. We present more additional case studies in Appendix B.1.

From the case study shown in Figure 3, we have the following observations. **First,** our system demonstrates superior performance in generating reasonable high-level hypotheses. For instance, when presented with the weight minimization problem, our fine-tuned foundation model directly proposed the octet lattice structure, recognizing its optimal stretch-dominated configuration and superior strength-to-weight ratio. In contrast, GPT-4o initially suggested a Body-Centered Cubic (BCC) configuration, which is less optimal for this specific application. This comparison highlights our model's enhanced domain knowledge and reasoning capabilities. **Second,** our system can effectively leverage human feedback and supplementary materials to improve hypothesis quality. When provided with expert feedback emphasizing "*use the most efficient lattice structures with high stiffness and strength*" and relevant research papers (e.g., Zheng et al. (2014) and Deshpande et al. (2001)), GPT-4o successfully revised its hypothesis from BCC to the more suitable octet-truss structure. The retrieved papers and text materials can also provide important references for our system to predict reasonable and valid ranges for the lattice properties in the fine-grained hypothesis. **Third,** we demonstrate that our system can generate valid 3D lattice structure and our refinement model can effectively refine and improve the generated structure. From Figure 3, the initial generated structure, while reasonable, showed slight asymmetries in its lattice properties. Through our refinement process, the structure was optimized to achieve better cubic symmetry with improved Young's modulus in the z axis. These improvements enhanced load distribution and reduced stress concentration points, resulting in superior overall strength and stiffness in the final design.

To verify the effectiveness of the design generated by METASCIENTIST, we 3D printed the lattice design using a Formlabs 3D printer and show that the 5 cm octet lattice cube can successfully support

	Novelty		Feasibility	
	Mean	Std	Mean	Std
GPT-4o	0.803	0.481	**1.591**	0.605
METASCIENTIST				
- w/o Human	0.833	0.582	1.227	0.651
- w/ Human	**1.712**	0.424	1.47	0.499

Table 1: Hypothesis Evaluation for **Novelty** and **Feasibility**. Each evaluation aspect has three scales, where score 0 is the worst and score 2 is the best.

Category	Error Threshold	Intra-cell Validity	Inter-cell Validity
Initial Lattice	0.005	22	0
	0.01	93	41
	0.02	97	82
	0.04	98	98
Refined Lattice	0.005	55	39
	0.01	94	52
	0.02	98	83
	0.04	98	98

Table 2: **Validity (%)** of the initially generated lattice structure and refined lattice structure.

a load of 10 kg without crushing. We included the images of the 3D printed structures in Figure 7 in the Appendix. These results demonstrate that our METASCIENTIST, encompassing hypothesis generation, lattice structure synthesis and refinement, can produce valid metamaterials in practical applications.

Quantitative Evaluation We also conduct quantitative experiments to evaluate textual hypothesis generation in Table 1, and 3D structure generation and refinement in Table 2. For hypothesis generation evaluation, we employ two widely adopted aspects, i.e., *novelty* and *feasibility* (Si et al., 2024). We test our system on 11 metamaterial research questions carefully curated by domain experts, and ask three senior researchers (i.e., 1 professor and 2 postdocs) in material science to evaluate the hypotheses generated by GPT-4o and our METASCIENTIST with or without human feedback. We include more details including evaluation criteria and the results for each instance in Appendix B.2. From the results in Table 1 and the comments from the human evaluators, we have the following findings: (1) The novelty and feasibility of the hypotheses generated by METASCIENTIST can be significantly improved after incorporating human feedback. Our approach outperforms the GPT-4o baseline in terms of novelty by a substantial margin while maintaining a competitive result in feasibility. (2) GPT-4o's hypotheses, while easier to complete and thus having a higher feasibility score, tend to be more trivial and lack the depth required for truly novel or ambitious ideas. In contrast, METASCIENTIST with human feedback produces hypotheses that are more complex and innovative, which inherently makes them more challenging to implement and leads to a slightly lower feasibility score.

For 3D structure validation, we design two metrics: *intra-cell validity* and *inter-cell validity*. There are two requirements for a structure to be intra-cell valid: all vertices should be connected and the structure should be symmetric, which means for each vertex, there should be a counterpart vertex for it, to make up a symmetric pair. To assert whether a structure is inter-cell valid, we first find a cubic frame corresponding to the unit cell of the structure, and then test whether any vertices exceed the boundary of the cubic frame. If not, the structure is considered to be inter-cell valid. Since the structures generated or refined are not perfectly precise, we allow the vertices to deviate slightly from their supposed location. A series of error thresholds (from 0.005 to 0.04) are set for the evaluation of structures. For each threshold, if a vertex suffers a deviation of more than the cell size times the threshold, then the structure is determined to be intra-cell or inter-call invalid. From Table 2 it can be observed that as the threshold increases, the validity also increases. If a relative error of 0.03 is allowed, then the majority of generated structures will be valid. Refined structures also show a similar pattern, but convergence will be reached with a lower threshold, which verifies the effectiveness of the refinement step.

4 Related Works

Automated scientific discovery has progressed significantly given the recent advancements of large foundation models (LLMs) (Wang et al., 2023; Lu et al., 2024; Papadimitriou et al., 2024; Xiong et al., 2024; Fu et al., 2024; Ishikawa, 2024; Du et al., 2024), such as logical reasoning (Sun et al., 2024), multi-agent collaboration (Ma et al., 2024; Jansen et al., 2024; Baek et al., 2024; Arawjo et al., 2024), automatic evaluation (Zheng et al., 2023; Liu et al., 2024a,b; Si et al., 2025), and tool and retrieval-based augmentation (Prince et al., 2024; Qi et al., 2024; Huang et al., 2024). However, the application of AI and LLMs for autonomous novel material discovery faces several challenges, including high error rates and hallucinations (Lehr et al., 2024; Miret and Krishnan, 2024), lacking interpretability (Liu et al., 2024c; Lei et al., 2024), rigorous logical and mathematical reasoning capabilities (Park et al., 2024; Deb et al., 2024; Zhang et al., 2024a), leading to scientifically unsound or unverifiable hypotheses. Additionally, LLMs often struggle to extrapolate beyond existing knowledge due to the nature of their pre-training objective (Petroni et al., 2019; Achiam et al., 2023). To address these challenges, METASCIENTIST employs a human-in-the-loop approach to integrate expert feedback and domain-specific knowledge into the design of novel materials, which significantly mitigates hallucinations and aligns outputs with scientific principles.

5 Conclusion

We propose METASCIENTIST that accelerates the discovery of novel metamaterials by integrating advanced AI capabilities with expert oversight. Experiments and human evaluation demonstrate that METASCIENTIST can generate reasonable and valid metamaterial design given the user's research question. Future works include improving the validity of lattice properties using more advanced retrieval techniques and building more powerful models to generate 3D metamaterial structures in more diverse scenarios. We believe our work has significant potential to advance the field of metamaterial design and other broad scientific domains.

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A More Implementation Details of METASCIENTIST

A.1 Foundation Model for Metamaterials Science

A.1.1 Data Collection

To construct a high-quality dataset for metamaterials science, we first ask a domain expert to provide a list of keywords related to metamaterial design, retrieve and download around 5,000 research papers and books in `PDF` format from Google Scholar. We then utilize specialized toolkits, including `pdfplumber`[8], `PyPDF2`[9] and `pdfminer`[10], combined with GPU-accelerated parsing[11] to convert the `PDF` documents to plaintext. To ensure the quality of the extracted text, we further employ rule-based filtering and natural language processing techniques to remove conversion errors, irrelevant content, and noise from the text. Specifically, we begin by leveraging regular expressions to identify and eliminate formatting errors, symbolic noise, and other low-quality elements in the extracted text. Subsequently, natural language processing tools such as SpaCy[12] and NLTK[13] are employed for sentence segmentation, enabling the removal of incoherent or contextually irrelevant fragments. Finally, we utilize text similarity algorithms (Reimers and Gurevych, 2019; Gao et al., 2021) to detect and remove redundant paragraphs and sentences, ensuring the uniqueness and relevance of processed text.

Finally, we categorize the cleaned text corpus into two subsets: (1) A **domain-specific** subset that includes academic papers and textbooks specifically focused on metamaterials science. Accounting for 80% of the whole training corpus, this subset provides specialized knowledge and ensures a deep focus on the target domain. (2) A **general-domain** subset that contains scientific papers about other topics in materials science and accounts for 20% of the training corpus. This subset offers foundational knowledge about the board materials science field, complementing the domain-specific insights. Table 3 shows detailed statistics of the dataset.

Category	Count	Details
Total pdf Files	5611	Approximately 480 Books
Domain-Specific Papers	4470	MetaMaterial Science
General-Domain Papers	1141	General Material Science
Converted `txt` Files	4711	After conversion
Words in Cleaned Data	42,488,911	(42M)
Tokens in Cleaned Data	74,814,532	(74M)

Table 3: Dataset Statistics for the Foundation Model

A.1.2 Model Training and Evaluation

The model was trained using a learning rate of 2×10^{-4} and the `Adam` optimizer (Kingma, 2014) with $\epsilon = 1 \times 10^{-8}$. A cosine learning rate scheduler was employed, with a warmup ratio of 0.1. For fine-tuning, we utilized LoRA with `lora_alpha=8` and a dropout rate of 0.05. The training was conducted on 4× RTX A6000 GPUs. To ensure optimal performance, models were trained across different numbers of epochs, and the version trained for 5 epochs was selected as the final iteration.

Comparison of Foundation model and Llama 3-8B As shown in Figure 4, the comparison highlights the differences in the responses generated by the Foundation Model (Ours) and the baseline LLaMA3-8B-Instruct model for material science-related questions. The Foundation Model exhibits a more detailed and contextually grounded understanding, integrating advanced scientific concepts such as the negative material index and the Hashin-Shtrikman bounds. Additionally, it provides clear examples of biological metamaterials, including the exoskeleton of the crab and the shell of the abalone, demonstrating a deeper domain-specific reasoning capability.

In contrast, the responses from the LLaMA3-8B-Instruct model are either overly generalized, repetitive, or lack sufficient scientific detail to address the questions effectively. This qualitative comparison underscores the improved performance of the Foundation Model in tasks requiring domain knowledge and contextual comprehension.

A.2 Hypothesis Generation

More details on Inductive Biases Extraction We let a domain expert in metamaterial science domain curate a metamaterial taxonomy for eliciting internal relevant knowledge from LLMs as shown in Figure 5 and Figure 6.

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[8] https://github.com/jsvine/pdfplumber

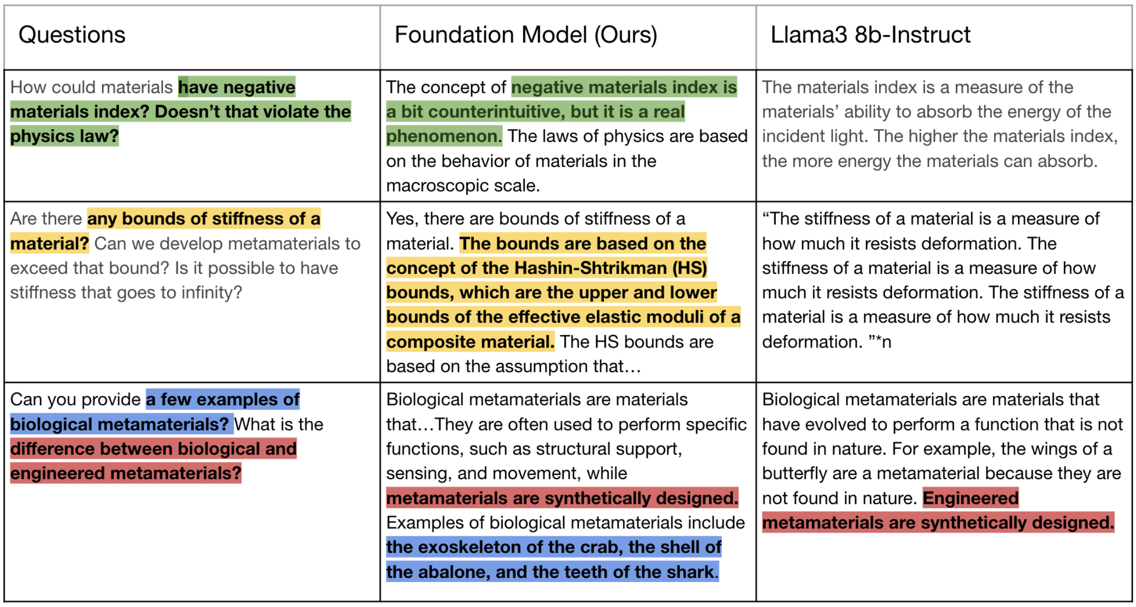
[9] https://github.com/py-pdf/pypdf

[10] https://github.com/pdfminer/pdfminer.six

[11] https://github.com/huridocs/pdf-document-layout-analysis

[12] https://spacy.io/

[13] https://www.nltk.org/



Questions	Foundation Model (Ours)	Llama3 8b-Instruct
How could materials **have negative materials index? Doesn't that violate the physics law?**	The concept of **negative materials index is a bit counterintuitive, but it is a real phenomenon.** The laws of physics are based on the behavior of materials in the macroscopic scale.	The materials index is a measure of the materials' ability to absorb the energy of the incident light. The higher the materials index, the more energy the materials can absorb.
Are there **any bounds of stiffness of a material?** Can we develop metamaterials to exceed that bound? Is it possible to have stiffness that goes to infinity?	Yes, there are bounds of stiffness of a material. **The bounds are based on the concept of the Hashin-Shtrikman (HS) bounds, which are the upper and lower bounds of the effective elastic moduli of a composite material.** The HS bounds are based on the assumption that…	"The stiffness of a material is a measure of how much it resists deformation. The stiffness of a material is a measure of how much it resists deformation. The stiffness of a material is a measure of how much it resists deformation. "*n
Can you provide **a few examples of biological metamaterials?** What is the **difference between biological and engineered metamaterials?**	Biological metamaterials are materials that…They are often used to perform specific functions, such as structural support, sensing, and movement, while **metamaterials are synthetically designed.** Examples of biological metamaterials include **the exoskeleton of the crab, the shell of the abalone, and the teeth of the shark.**	Biological metamaterials are materials that have evolved to perform a function that is not found in nature. For example, the wings of a butterfly are a metamaterial because they are not found in nature. **Engineered metamaterials are synthetically designed.**

Figure 4: Comparison of answers provided by the Foundation Model (Ours) and LLaMA3-8B-Instruct to questions about material science.

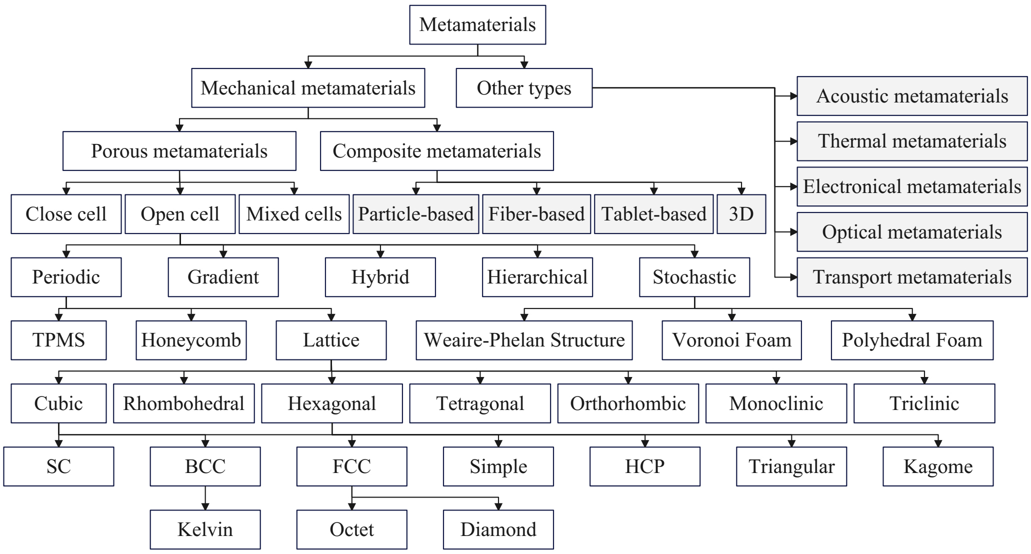


Figure 5: Illustration of our curated taxonomy tree in mechanical metamaterials used in internal inductive bias extraction.

A.3 3D Structure Synthesis

Training Details for 3D Structure Generation

To train our 3D structure synthesis models, we extend the Modulus (Lumpe and Stankovic, 2021) dataset by applying scaling and rotation transformations to its lattice topologies, paired with adjusted lattice properties to ensure the dataset captures a broader range of variations. During training, the diffusion block receives 3D coordinates mixed with Gaussian noise as input, along with the corresponding lattice properties as conditioning information. The model predicts the clean 3D coordinates in a single step, and the loss is computed based on the difference between the predicted and ground truth coordinates. Simultaneously, the edge prediction block is trained by comparing its predictions with ground truth vertex connections. This joint training process enables the model to generate accurate and structurally coherent 3D lattice designs.

Training Details for 3D Structure Refinement

The major difficulty in training the refinement model is the limited availability of paired data showing both unrefined and properly refined lattice structures. While researchers typically publish

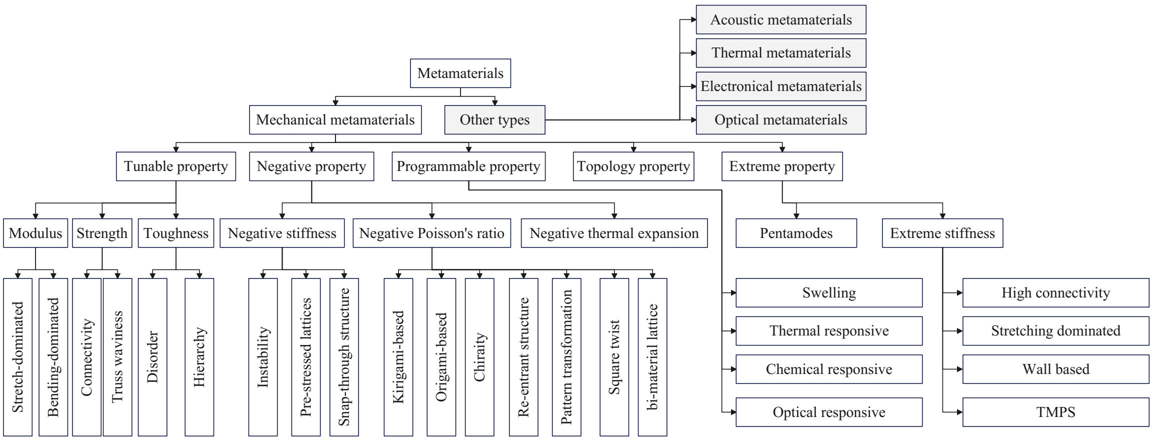


Figure 6: Illustration of our curated taxonomy tree in mechanical metamaterials used in internal inductive bias extraction.

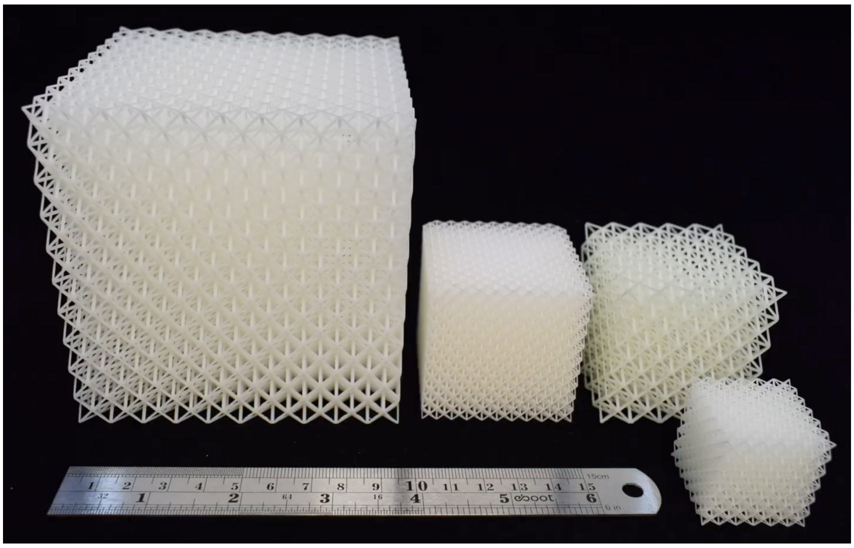


Figure 7: 3D-printed lattice structures from our generated hypothesis. These lattice structures have sizes of 10 cm, 5 cm, 5 cm, and 3 cm, respectively.

only their optimized final structures, they often omit documenting the optimization process itself. To overcome this obstacle, we synthesize training data based on the Unit Cell Catalog (Lumpe and Stankovic, 2021). The diffusion-generated lattices exhibited two primary failure patterns: inaccurate node coordinates and incorrect node/edge configurations (either missing or excessive). To mimic these failure patterns, we corrupt the perfect lattice by randomly remove or add nodes and edges, and inject Gaussian noise into the node coordinates. Hereafter, we supervised finetune the pretrained model (Llama-3.1-8B-Instruct (Dubey et al., 2024)) by fitting the lattice structure information into the prompt and response template. The model gets the corrupted lattice in the prompt and is trained to include the perfect lattice in the response.

B More Experiment Details and Results

B.1 Case Studies

We present additional case studies in Figure 8. From this case study focusing on designing a lattice structure for a robotic fingertip that mimics human hand properties, we have the following observations. **First,** our system effectively incorporates domain expertise through human feedback and supplementary materials. Though our fine-tuned foudation model proposed a more sophisticated hierarchical octet topology with gradient volume fraction, when provided with expert feedback emphasizing high stiffness and strength requirements, along with relevant papers on human finger pad mechanics and 3D lattice structures, our systems converged on the Kelvin cell configuration focusing primarily on isotropy. The supplementary materials also helped establish reasonable ranges for mechanical properties in the fine-grained hypothesis, particularly in matching human tissue characteristics. **Second,** we demonstrate that our refinement model can successfully optimize the generated lattice structure for improved mechanical symmetry. The initial structure showed variations in Young's modulus (ranging from 3.00e-02 to 3.79e-02) and significant anisotropy in Poisson ratios (ranging from 4.23e-02 to 2.02e-01). Through our refinement process, these properties were harmonized to achieve perfect cubic symmetry with consistent values (Young's modulus of 3.19e-02 and Poisson ratio of 2.97e-01).

B.2 More Details and Results of Human Evaluation for Hypothesis Generation

Human Evaluation We evaluate the generated hypotheses with two aspects, i.e., *novelty* and *feasibility*. We ask three senior researchers in the metamaterial domain as the reviewers to score the system-generated hypotheses. Each reviewer gives the scores independently. The evaluation criteria are defined as follows:

Novelty: Whether the idea is creative and different from existing works on the topic, and brings fresh insights.

- **Score 0 (Low Novelty):** The idea closely resembles many existing works with minimal differentiation.
- **Score 1 (Medium Novelty):** The idea shows some differences from existing works but has obvious overlaps with prior concepts.
- **Score 2 (High Novelty):** The idea introduces major differences, offering distinct insights or approaches absent in existing works.

Feasibility: How feasible is it to implement and execute this idea as a research work.

- **Score 0 (Low Feasibility):** The idea is highly impractical or requires resources/techniques currently unavailable.
- **Score 1 (Medium Feasibility):** The idea is somewhat practical but faces notable challenges in execution or resource availability.
- **Score 2 (High Feasibility):** The idea is practical and can be implemented with available resources and techniques.

The complete list of the examples used in human evaluation can be found in Appendix D.

C Prompts used in METASCIENTIST

We offer all prompts we used in the METASCIENTIST in Figure 9, 10, and 11.

Case Study 2

Input research question:

Our task is to design a lattice structure for the fingertip of a robotics hand with the size of a human hand. We need to determine what material, lattice unit cell, and volume fraction to use. Note that we want the lattice structure-based fingertip to have mechanical properties close to that of an actual human hand and is capable of having large deformation repeatedly. The designed lattice structure will be printed by a Formlab 3D printer.

Generated high-level hypothesis:

from GPT-4o:

In addressing the challenge of designing a lattice structure for the fingertip of a robotic hand that mimics the mechanical properties of a human hand, we propose the development of a periodic open-cell lattice structure utilizing a **Kelvin cell configuration**. The Kelvin cell, known for its isotropic mechanical properties and efficient space-filling capability, offers a promising foundation for achieving the desired balance between stiffness and flexibility.

from our foundation model:

In response to the challenge of designing a lattice structure for the fingertip of a robotics hand that emulates the mechanical properties and deformation capabilities of a human hand, we propose the development of a hierarchical, open-cell lattice structure based on the **octet topology**, combined with a gradient volume fraction approach. The motivation for this hypothesis lies in the need to achieve a balance between strength and flexibility, essential for replicating the nuanced mechanical behavior of human skin and soft tissue.

Supplementary material:

- *Human feedback:* Please use the most efficient lattice structures, i.e., high stiffness and strength.
- *Papers:* [1] Contact mechanics of the human finger pad under compressive loads" by Dzidek et al. [2] Design of a Reconfigurable Modular Chain for Folding 3D Lattice Structures by Zhe Xu et al.
- *Textual materials: [1]* Kelvin Cell Topology. The Kelvin cell topology is a type of closed-cell ... [2] Hierarchical Lattice Structures. Hierarchical lattice structures incorporate multiple scales of architecture ...

Generated fine-grained hypothesis (from GPT-4o):

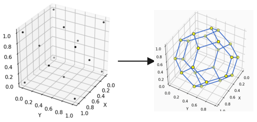
To design a lattice structure for the fingertip of a robotic hand that mimics the mechanical properties of a human hand, we propose the development of a periodic open-cell lattice structure utilizing a Kelvin cell configuration. The **Kelvin cell**, known for its isotropic mechanical properties and efficient space-filling capability, offers a promising foundation for achieving the desired balance between stiffness and flexibility. The lattice will be constructed with a unit cell composed of a truncated octahedron, where each node is connected by struts of uniform cross-section, ensuring isotropic behavior. The struts will be designed with a diameter of 0.5 mm, and the overall cell size will be 5 mm, allowing for a volume fraction of approximately 30%. This configuration is selected to optimize energy absorption and resilience while maintaining structural integrity. By selecting a photopolymer resin compatible with Formlab 3D printers, we can ensure the material's suitability for repeated large deformations, akin to the tactile and elastic characteristics of human skin. The resin will be engineered to achieve a Young's modulus of approximately 1.0 GPa, a shear modulus of 0.8 GPa, and a Poisson's ratio of 0.3, reflecting the isotropic nature of the Kelvin cell. This approach leverages the inherent advantages of the Kelvin cell's geometry, which facilitates uniform stress distribution and minimizes localized deformation, thereby enhancing durability and functionality. Through this design, we aim to achieve a robotic fingertip that not only replicates the tactile feedback and dexterity of a human hand but also withstands the rigors of repetitive mechanical loading.

Generated Lattice Properties for conditional 3D Structure Generation:

- Young modulus: [1.00e-03, 1.10e-03, 1.20e-03]
- Shear modulus: [8.00e-04, 8.50e-04, 9.00e-04]
- Poisson ratio: [3.00e-01, 3.20e-01, 3.40e-01, 3.10e-01, 3.30e-01, 3.50e-01]

Generated 3D lattice structure:

- Young modulus: [3.79e-02, 3.00e-02, 3.25e-02]
- Shear modulus: [1.67e-02, 1.29e-02, 1.43e-02]
- Poisson ratio: [2.02e-01, 1.60e-01, 4.23e-02, 4.58e-02, 1.58e-01, 1.84e-01]



Refined 3D lattice structure:

- Young modulus: [3.19e-02, 3.19e-02, 3.19e-02]
- Shear modulus: [6.57e-03, 6.57e-03, 6.57e-03]
- Poisson ratio: [2.97e-01, 2.97e-01, 2.97e-01, 2.97e-01, 2.97e-01, **2.97e-01**]

The refined version adjusts the node coordinates to remove slight asymmetries. The **enhanced symmetry** results in a more uniform load distribution, which reduces stress concentration points and potential failure spots.

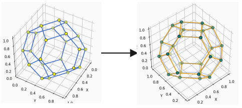


Figure 8: **Case study** of *designing a lattice structure for the fingertip of a robotics hand* using METASCIENTIST.

LLM Prompts 1

Generate high-level hypothesis

~~~~
**Context**
I am a researcher specializing in mechanical metamaterials. I am tasked with generating hypotheses that serve as solutions or answers to specific research questions.

**Objective**
Your role is to help me develop a hypothesis in response to a given question. The hypothesis should be structured as a formal academic proposal paragraph, providing the motivation and the main concept of the proposed approach.

**Style**
Maintain a formal, professional tone consistent with academic writing in the field of mechanical metamaterials.

**Hints**
You may refer to the following taxonomy for inspiration in generating the hypothesis.

*Taxonomy (Structure-based):*
[1] Closed cell [2] Mixed cell [3] Open cell [3.1] Periodic [3.1.1] TPMS [3.1.2] Honeycomb [3.1.3] Lattice [3.1.4] Cubic [3.1.5] SC [3.1.6] BCC [3.1.7] Kelvin [3.1.8] FCC [3.1.9] Octet [3.1.10] Diamond [3.1.11] Rhombohedral [3.1.12] Hexagonal [3.1.13] Simple [3.1.14] HCP [3.1.15] Triangular [3.1.16] Kagome [3.1.17] Tetragonal [3.1.18] Orthorhombic [3.1.19] Monoclinic [3.1.20] Triclinic [3.2] Gradient [3.3] Hybrid [3.4] Hierarchical [3.5] Stochastic [3.5.1] Weaire-Phelan Structure [3.5.2] Voronoi Foam [3.5.3] Polyhedral Foam

*Taxonomy (Design-based):*
[1] Tunable property [1.1] Modulus [1.1.1] Stretch-dominated [1.1.2] Bending-dominated [1.2] Strength [1.2.1] Connectivity [1.2.2] Truss waviness [1.3] Toughness [1.3.1] Disorder [1.3.2] Hierarchy [2] Negative property [2.1] Negative stiffness [2.1.1] Instability [2.1.2] Pre-stressed lattices [2.1.3] Snap-through structure [2.2 Negative Poisson's ratio [2.2.1] Kirigami-based [2.2.2] Origami-based [2.2.3] Chirality [2.2.4] Re-entrant structure [2.2.5] Pattern transformation [2.2.6] Square twist [2.3 Negative thermal expansion [2.3.1] Bi-material lattice [3] Programmable property [3.1] Swelling [3.2] Thermal responsive [3.3] Chemical responsive [3.4] Optical responsive [4] Extreme property [4.1] Pentamodes [4.2] Extreme stiffness [4.2.1] High connectivity [4.2.2] Stretch-dominated [4.2.3] Wall-based [4.2.4] TPMS [5] Topology property

**Response**
The hypothesis should be presented in a formal, professional tone, grounded in the science of mechanical metamaterials. It should resemble a paragraph from an academic proposal, addressing the motivation and main idea of the proposed approach as a solution to the given question. In addition, estimate your confidence in this hypothesis (in high, midden, low), where high means you believe this hypothesis is definitely correct and feasible; low indicates that this hypothesis is merely a guess and is most likely incorrect.
Here is a response example:
```json
{
   "hypothesis": "a paragraph of hypothesis",
   "confidence": "high/midden/low"
}
```
PS: Avoid using the hybrid lattice structure or structure ensemble strategy.

**Question**
<|question|>

**Hypothesis**
~~~~

Answer sub-questions

~~~~
**Context**
I am a researcher specializing in mechanical metamaterials.

**Objective**
Your role is to help me answer research questions.

**Question**
<|question|>

**Answer**
~~~~

Raise sub-questions

~~~~
**Context**
I am a researcher specializing in mechanical metamaterials. I am tasked with parsing and decomposing complex research questions.

**Objective**
Your role is to help me raise several sub-questions to a given question. The answers to these raised should be able to provide more information to help me solve the original question.

**Hints**
You may refer to the following taxonomy for inspiration in generating the sub-quesions.

*Taxonomy (Structure-based):*
[1] Closed cell [2] Mixed cell [3] Open cell [3.1] Periodic [3.1.1] TPMS [3.1.2] Honeycomb [3.1.3] Lattice [3.1.4] Cubic [3.1.5] SC [3.1.6] BCC [3.1.7] Kelvin [3.1.8] FCC [3.1.9] Octet [3.1.10] Diamond [3.1.11] Rhombohedral [3.1.12] Hexagonal [3.1.13] Simple [3.1.14] HCP [3.1.15] Triangular [3.1.16] Kagome [3.1.17] Tetragonal [3.1.18] Orthorhombic [3.1.19] Monoclinic [3.1.20] Triclinic [3.2] Gradient [3.3] Hybrid [3.4] Hierarchical [3.5] Stochastic [3.5.1] Weaire-Phelan Structure [3.5.2] Voronoi Foam [3.5.3] Polyhedral Foam

*Taxonomy (Design-based):*
[1] Tunable property [1.1] Modulus [1.1.1] Stretch-dominated [1.1.2] Bending-dominated [1.2] Strength [1.2.1] Connectivity [1.2.2] Truss waviness [1.3] Toughness [1.3.1] Disorder [1.3.2] Hierarchy [2] Negative property [2.1] Negative stiffness [2.1.1] Instability [2.1.2] Pre-stressed lattices [2.1.3] Snap-through structure [2.2 Negative Poisson's ratio [2.2.1] Kirigami-based [2.2.2] Origami-based [2.2.3] Chirality [2.2.4] Re-entrant structure [2.2.5] Pattern transformation [2.2.6] Square twist [2.3 Negative thermal expansion [2.3.1] Bi-material lattice [3] Programmable property [3.1] Swelling [3.2] Thermal responsive [3.3] Chemical responsive [3.4] Optical responsive [4] Extreme property [4.1] Pentamodes [4.2] Extreme stiffness [4.2.1] High connectivity [4.2.2] Stretch-dominated [4.2.3] Wall-based [4.2.4] TPMS [5] Topology property

**Response**
Here is a response example:
```json
{
   "sub-question 1": "a sub-question",
   "sub-question 2": "another sub-question"
}
```
PS: you can raise a maximum of five sub-questions.

**Question**
<|question|>

**Answer**
~~~~

Incorporate human feedback for high-level hypothesis

~~~~
## Context ##
I am a researcher in the field of mechanical metamaterials, currently working on refining a research hypothesis. I have received feedback from an expert in the field, along with additional relevant materials. My goal is to revise the hypothesis so that it addresses the research question effectively while aligning with the preferences and insights provided by the expert.

## Objective ###
Your task is to incorporate the expert feedback and any additional material (if applicable) to revise and refine the hypothesis. The revised hypothesis should represent a sound solution to the research question, aligning with human preferences. It should be written in a formal academic style and presented as a paragraph suitable for inclusion in a professional research proposal. This paragraph should clearly convey the motivation for the research and the main idea of the proposed approach.

## Style ##
The response should be formal, professional, and aligned with the conventions of mechanical metamaterial science.

## Response ##
Please ensure that the revised hypothesis fully considers the expert's feedback and integrates any additional material provided. The response should be written in a formal academic tone and structured as a cohesive paragraph from a research proposal. It should clearly articulate the motivation behind the approach and how it addresses the research question.
PS: Avoid using the hybrid lattice structure or structure ensemble strategy.

## Task inputs ##
<---Question--->
<|question|>
<---Current hypothesis--->
<|hypothesis|>
<---Human expert feedback--->
<|feedback|>
<---Additional material--->
<|material|>
<---Reference paper--->
<|paper|>
<---Conversation with Domain Expert--->
<|chat|>

**Modified Hypothesis**
~~~~

Figure 9: Prompts used in METASCIENTIST (part 1)

LLM Prompts 2

Generate fine-grained hypothesis

Context
I am a researcher specializing in mechanical metamaterials, tasked with refining a hypothesis to a detailed level that directly addresses specific research questions.

Objective
Your role is to help me fine-tune this hypothesis into a highly specific material structure design.
First, you need to help me revise the given hypothesis and fine-grained it to a more detailed level. It should talk about the specific design of this lattice structure, e.g., what structure is in each layer, how nodes connect in the unit cell, etc. In addition, this refined design should include precise values for Young's modulus, Shear modulus, and Poisson's ratio, so that I can know the expected property of this lattice.
Second, list the estimated Young's modulus, Shear modulus and Poisson's ratio in another paragraph. I will show you two examples to demonstrate the specific output format.
The hypothesis should be formal, clear, and well-structured, presenting both the theoretical and implementation details of the proposed approach with designated values for each of the three modules.

Style
Maintain a formal, academic tone suitable for research in mechanical metamaterials. Instead of summarizing the properties or providing an introductory overview, provide detailed explanations of the design concepts. For example, rather than describing a structure as “a hybrid lattice combining octet truss and rhombohedral configurations,” explain precisely how these structures are combined, how the lattice connection is designed, and how hierarchical design strategies contribute to material enhancement.

Response Structure
The hypothesis has to be returned in JSON format and include two sections:
1. **Hypothesis**: A paragraph that reads as if from an academic proposal, outlining the motivation and details of the proposed approach as a solution to the given research question.
2. **Lattice Properties**: A JSON object with three key-value pairs for the material’s mechanical properties:
  - **Young_module**: [value1, value2, value3]
  - **Shear_module**: [value1, value2, value3]
  - **Poisson_module**: [value1, value2, value3, value4, value5, value6]
3. Estimate your confidence in this hypothesis (in high, midden, low), where high means you believe this hypothesis is definitely correct and feasible; low indicates that this hypothesis is merely a guess and is most likely incorrect.

Examples
Example 1:
```json
{
   "hypothesis": "To xxxxxx, we need to xxxxxx. Based on material xxxxxxx, xxxxxx can be inferred. A possible solution is xxxxxx, which could yield xxxxxx material properties. The lattice structure should therefore be xxxxxx.",
   "lattice": {
      "Young_module": [1.58e-03,1.37e-03,9.73e-04],
      "Shear_module": [1.19e-03,6.93e-04,1.03e-03],
      "Poisson_module": [4.75e-01,2.96e-01,3.12e-01,0.27e-01,3.75e-01,4.37e-01]
   },
"confidence": "high"
}
```
Example 2:
```json
{
   "hypothesis": "xxxxxx is a potential way to xxxxxx. Current limitations in xxxxxx suggest that the lattice should meet xxxxxx requirements. Furthermore, it should exhibit xxxxxx properties. With this design, the material could achieve xxxxxx characteristics.",
   "lattice": {
      "Young_module": [1.58e-03,1.37e-03,9.73e-04],
      "Shear_module": [1.19e-03,6.93e-04,1.03e-03],
      "Poisson_module": [4.75e-01,2.96e-01,3.12e-01,0.27e-01,3.75e-01,4.37e-01]
   },
"confidence": "low"
}
```

Constraints
Avoid using the hybrid lattice structure or structure ensemble strategy.

Input
Question
<|question|>

Current Hypothesis
<|hypothesis|>

Supporting Material
<---Additional material--->
<|material|>
<---Reference paper--->
<|paper|>

Deliverable

Incorporate human feedback for fine-grained hypothesis

Context
I am a researcher specializing in mechanical metamaterials, working to refine a research hypothesis based on feedback from an expert in the field. I also have access to additional relevant materials. My goal is to revise the hypothesis so that it effectively addresses the research question while incorporating the expert's insights and preferences.

Objective
Your task is to use the expert feedback and any applicable additional materials to revise and refine the hypothesis. The revised hypothesis should present a well-defined solution aligned with the research question and adhere to human preferences. The design must include specific values for the Young’s modulus, Shear modulus, and Poisson’s ratio, with a formal, clear, and well-structured approach detailing both theoretical and implementation aspects of the solution.

Style
The response should maintain a formal, academic tone appropriate for the field of mechanical metamaterials.

Response Format
The output has to be in JSON format, consisting of two sections:

1. **Hypothesis**: A paragraph that would fit within an academic proposal, detailing the motivation and implementation specifics of the proposed solution to the research question.
2. **Lattice Properties**: A JSON object including the following key-value pairs, where values represent the proposed design parameters for the material:
  - **Young_module**: [value1, value2, value3]
  - **Shear_module**: [value1, value2, value3]
  - **Poisson_module**: [value1, value2, value3, value4, value5, value6]

Example Responses
Example 1:
```json
{
   "hypothesis": "To xxxxxx, we need to xxxxxx. Based on material xxxxxxx, xxxxxx can be inferred. A possible solution is xxxxxx, which could yield xxxxxx material properties. The lattice structure should therefore be xxxxxx.",
   "lattice": {
      "Young_module": [1.58e-03,1.37e-03,9.73e-04],
      "Shear_module": [1.19e-03,6.93e-04,1.03e-03],
      "Poisson_module": [4.75e-01,2.96e-01,3.12e-01,0.27e-01,3.75e-01,4.37e-01]
   }
}
```
Example 2:
```json
{
   "hypothesis": "xxxxxx is a potential way to xxxxxx. Current limitations in xxxxxx suggest that the lattice should meet xxxxxx requirements. Furthermore, it should exhibit xxxxxx properties. With this design, the material could achieve xxxxxx characteristics.",
   "lattice": {
      "Young_module": [1.58e-03,1.37e-03,9.73e-04],
      "Shear_module": [1.19e-03,6.93e-04,1.03e-03],
      "Poisson_module": [4.75e-01,2.96e-01,3.12e-01,0.27e-01,3.75e-01,4.37e-01]
   }
}
```

Constraints
Avoid using the hybrid lattice structure or structure ensemble strategy.

Inputs
- *Question*: <|question|>
- *Current Hypothesis*: <|hypothesis|>
- *Expert Feedback*: <|feedback|>
- *Additional Material*: <|material|>
- *Reference paper*:
<|paper|>
<---Conversation with Domain Expert--->
<|chat|>

Deliverable

Figure 10: Prompts used in METASCIENTIST (part 2)

LLM Prompts 3

Retreival for inductive bias

~~~~
**Context**
I am a researcher in mechanical metamaterials, working on a literature review for a specific research question and hypothesis provided by experts in the field. My goal is to gather existing knowledge and relevant materials that inform this hypothesis.

**Objective**
Your task is to help me compile a list of known materials, lattice structures, or approaches relevant to the hypothesis. For each item, include its attributes, properties, and any specific values for Young’s modulus, Shear modulus, and Poisson’s ratio, if available.

**Hints**
You may refer to the following taxonomy for inspiration in generating the sub-quesions.

*Taxonomy (Structure-based):*
[1] Closed cell [2] Mixed cell [3] Open cell [3.1] Periodic [3.1.1] TPMS [3.1.2] Honeycomb [3.1.3] Lattice [3.1.4] Cubic [3.1.5] SC [3.1.6] BCC [3.1.7] Kelvin [3.1.8] FCC [3.1.9] Octet [3.1.10] Diamond [3.1.11] Rhombohedral [3.1.12] Hexagonal [3.1.13] Simple [3.1.14] HCP [3.1.15] Triangular [3.1.16] Kagome [3.1.17] Tetragonal [3.1.18] Orthorhombic [3.1.19] Monoclinic [3.1.20] Triclinic [3.2] Gradient [3.3] Hybrid [3.4] Hierarchical [3.5] Stochastic [3.5.1] Weaire-Phelan Structure [3.5.2] Voronoi Foam [3.5.3] Polyhedral Foam

*Taxonomy (Design-based):*
[1] Tunable property [1.1] Modulus [1.1.1] Stretch-dominated [1.1.2] Bending-dominated [1.2] Strength [1.2.1] Connectivity [1.2.2] Truss waviness [1.3] Toughness [1.3.1] Disorder [1.3.2] Hierarchy [2] Negative property [2.1] Negative stiffness [2.1.1] Instability [2.1.2] Pre-stressed lattices [2.1.3] Snap-through structure [2.2 Negative Poisson's ratio [2.2.1] Kirigami-based [2.2.2] Origami-based [2.2.3] Chirality [2.2.4] Re-entrant structure [2.2.5] Pattern transformation [2.2.6] Square twist [2.3 Negative thermal expansion [2.3.1] Bi-material lattice [3] Programmable property [3.1] Swelling [3.2] Thermal responsive [3.3] Chemical responsive [3.4] Optical responsive [4] Extreme property [4.1] Pentamodes [4.2] Extreme stiffness [4.2.1] High connectivity [4.2.2] Stretch-dominated [4.2.3] Wall-based [4.2.4] TPMS [5] Topology property

**Response Format**
The output should be in JSON format as a list of knowledge items. Each entry should represent either a material, structure, approach, or other concept in mechanical metamaterials, structured as a dictionary with the following keys:
- **name**: The name of the material, structure, or concept.
- **description**: A brief description of the item, including its properties, structural composition, and any notable behaviors or applications.
- **value**: Values of specific modules (Young’s modulus, Shear modulus, Poisson’s ratio) as reported in the literature, if available.

**Example Responses**
Example 1:
```json
{
   "name": "xxx structure",
   "description": "The xxx structure is common in xxxxx. It typically consists of xxx and xxx components. Under compressive force, this structure dissipates force by xxxxx, enhancing the xxxx of the material. This structure is widely used in xxxxxx applications.",
    "value": "According to literature xxxxx, material xxx with an xxx structure has Young’s modulus = [0.00399, 0.00201, 0.00399], Shear modulus = [2.55e-06, 7.67e-06, 4.03e-06], and Poisson’s ratio = [0.0, 0.0, 0.0, 0.0, 0.0, 0.0]."
}
```
Example 2:
```json
{
   "name": "xxx material",
    "description": "The xxx material is a natural product of xxx with properties like xxx and attributes including xxx. These properties are largely due to xxxxx of the xxx. Inspired by this natural structure, industries have designed materials with similar lattice structures xxxxx, enhancing specific performance attributes.",
      "value": "According to literature xxxxx, material xxx with this lattice structure has Young’s modulus = [8.64e-06, 8.64e-06, 0.00199], Shear modulus = [0.000745, 0.000745, 0.00114], and Poisson’s ratio = [0.001, 0.001, 0.995, 0.325, 0.325, 0.995]. Another material with a similar structure has Young’s modulus = [0.00251, 0.00251, 0.00498], Shear modulus = [3.99e-06, 3.99e-06, 1.22e-06], and Poisson's ratio = [0.0, -0.0, 0.0, 0.0, -0.0, 0.0]."
}
```


**Inputs**
- *Question*: <|question|>
- *Current Hypothesis*: <|hypothesis|>

**Deliverable**
~~~~

Summarize paper

~~~~
**Context**
I am a researcher in mechanical metamaterials conducting a literature review to support a specific research question and hypothesis provided by experts. My objective is to gather relevant knowledge and materials that inform this hypothesis.

**Objective**
Your task is to help me extract and summarize content from a given paper that relates to the research question and hypothesis. If the paper discusses specific lattice structures or properties, such as Young’s modulus, Shear modulus, and Poisson’s ratio, please include these details in the response.

**Response Format**
The output should be a concise, cohesive paragraph summarizing the paper’s content relevant to the research question and hypothesis. If it is coherent, please cite the original sentence from the paper. Please use the examples below as a reference for structure and detail:

***Example Responses***

Example 1:
```
Paper <xxxxxxxx> focuses on xxxx. The xxx structure is prevalent in xxxxx applications and typically consists of xxx and xxx components. When subjected to compressive force, this structure dissipates energy through xxxxx, enhancing the material's xxxx properties. It is widely used in xxxxxx applications. The most common values for Young's modulus and Poisson's ratio for this structure are [xx, xx, xx, xx] and [xx, xx, xx, xx, xx, xx], respectively.
```
Example 2:
```
Paper <xxxxxxxx> explores the xxx material, a natural product of xxx with unique properties such as xxx and specific attributes like xxx. These properties stem from xxxxx of the xxx. Inspired by this natural structure, industries have developed materials with similar lattice configurations, enhancing performance attributes. Typical values for Young's modulus and Shear modulus of this material are [xx, xx, xx, xx] and [xx, xx, xx, xx, xx, xx].
```


**Inputs**
- **Research Question**: <|question|>
- **Hypothesis**: <|hypothesis|>
- **Relevant Paper**: ```
<|paper|>
```

**Refined Paper Content**
~~~~

Figure 11: Prompts used in METASCIENTIST (part 3).

D Examples for human evaluation

- **Example 1**
  - **Topic:** novel lattice metamaterials
  - **Question:** Can you propose a novel scientific hypothesis on designing lattice metamaterials that are drastically different from existing concepts? The concept should have solid reasoning, and the designs generated based on the hypothesis should be testable and can be easily manufactured.
  - **GPT-4o:**
    - **Hypothesis:** In the pursuit of designing lattice metamaterials that diverge significantly from existing concepts, we propose the development of a novel class of metamaterials based on a hierarchical, multi-scale approach that integrates periodic and stochastic elements. This innovative design paradigm leverages the inherent advantages of both periodic structures, such as TPMS and BCC lattices, and stochastic configurations like Voronoi foams, to achieve unprecedented mechanical properties. The motivation for this approach stems from the need to overcome the limitations of traditional lattice designs, which often exhibit trade-offs between strength, toughness, and manufacturability. By embedding stochastic elements within a periodic framework, we hypothesize that it is possible to enhance the energy absorption capacity and damage tolerance of the metamaterial while maintaining

structural integrity and ease of fabrication. This dual-scale design can be realized through advanced additive manufacturing techniques, which allow for precise control over the micro-architecture. The proposed metamaterials are expected to exhibit tunable mechanical properties, such as modulus and toughness, by adjusting the scale and distribution of the stochastic elements within the periodic matrix. This hypothesis not only provides a solid foundation for the development of next-generation metamaterials but also opens new avenues for experimental validation and practical applications in fields requiring lightweight, high-performance materials.

    - **Reviewer Comment:** Lack of novelty. The combination of periodic and stochastic structures in a dual-scale configuration is not explained.
    - **Novelty:** [0,1,1]
    - **Feasibility:** [1,2,2]
- **MetaScientist without human:**
    - **Hypothesis:** To address the challenge of designing lattice metamaterials that are drastically different from existing concepts, we propose a novel approach that leverages a dual-layered lattice structure with distinct mechanical properties. The design consists of a primary layer featuring a hexagonal close-packed (HCP) configuration, known for its high packing density and isotropic mechanical properties, and a secondary layer composed of a diamond cubic lattice, which provides excellent stiffness and low density. The nodes in the HCP layer are connected through cylindrical struts with a diameter of 0.5 mm, while the diamond cubic layer utilizes struts with a diameter of 0.3 mm. The integration of these two layers is achieved through a hierarchical interlocking mechanism, where the nodes of the diamond cubic lattice are embedded within the interstitial spaces of the HCP layer, ensuring seamless load transfer and enhanced structural integrity. This design is expected to exhibit a Young's modulus of approximately 1.1e-3, a shear modulus of 8.5e-4, and a Poisson's ratio of 0.32, providing a balance between stiffness, strength, and manufacturability. The proposed metamaterial can be fabricated using advanced additive manufacturing techniques, allowing for precise control over the micro-architecture and enabling the exploration of tunable mechanical properties by adjusting the relative thickness and orientation of the layers. This hypothesis not only offers a new direction for the development of next-generation metamaterials but also provides a testable and manufacturable solution for applications requiring lightweight, high-performance materials.
    - **Reviewer Comment:** Lack of novelty. How the two layers are connected at the interstitial of HCP layer is not clear.
    - **Novelty:** [0,1,0]
    - **Feasibility:** [1,1,2]
- **Metascientist with human:**
    - **Hypothesis:** In response to the challenge of designing lattice metamaterials that diverge significantly from existing paradigms, we propose a novel hypothesis centered on the integration of phase-change principles at the lattice structure level to enable dynamic adaptability. This approach is motivated by the need for metamaterials that can alter their mechanical properties in real-time to meet diverse application requirements, such as in aerospace components that adapt to varying flight conditions or biomedical devices that respond to physiological changes. By leveraging phase-change mechanisms within the lattice architecture itself, rather than at the material level, we can achieve reversible transformations in the structural configuration in response to external stimuli like temperature or electrical inputs. This structural phase-change capability allows for the modulation of mechanical properties, including stiffness, damping, and energy absorption, providing a versatile platform for tailored performance. The hypothesis posits that by strategically designing lattice geometries that can undergo controlled reconfiguration through localized heating or electrical activation, we can achieve a metamaterial system capable of transitioning between

    multiple functional states, thereby offering unprecedented adaptability. This concept not only aligns with current research trends but also opens new avenues for exploration in the field of mechanical metamaterials. The proposed designs are amenable to fabrication using contemporary additive manufacturing techniques, ensuring their feasibility and facilitating empirical validation.
    - **Reviewer Comment:** While the idea is still not new, using phase-change principles is interesting.
    - **Novelty:** [1,2,2]
    - **Feasibility:** [2,1,1]

- **Example 2**
  - **Topic:** ultra efficient structural materails
  - **Question:** Can you generate some really novel scientific hypotheses in how to improve the structural efficiency of lattice materials, which can be validated or falsified relatively easily by experiments, but are also quite interesting and important?
  - **GPT-4o:**
    - **Hypothesis:** In response to the question of improving the structural efficiency of lattice materials, we propose the hypothesis that incorporating a hierarchical design approach within a periodic open-cell lattice structure, specifically utilizing a combination of TPMS (Triply Periodic Minimal Surfaces) and octet truss configurations, can significantly enhance the mechanical performance of these materials. The motivation for this hypothesis stems from the inherent advantages of hierarchical structures, which are known to provide superior strength-to-weight ratios and energy absorption capabilities due to their multi-scale architecture. By integrating TPMS, known for its minimal surface area and high stiffness, with the octet truss, recognized for its stretch-dominated behavior, we anticipate achieving a synergistic effect that optimizes both stiffness and strength. This approach not only leverages the geometric complexity of TPMS to distribute stress uniformly but also utilizes the efficient load-bearing capacity of the octet truss. The proposed hypothesis can be validated through experimental fabrication and mechanical testing of lattice prototypes, assessing parameters such as compressive strength, stiffness, and energy absorption. This investigation holds significant potential for advancing the design of lightweight, high-performance materials in applications ranging from aerospace to biomedical engineering.
    - **Reviewer Comment:** Hierachy is a well known design stragety. Hierarchy does not necessarily improve the mechanical efficiency.
    - **Novelty:** [0,1,1]
    - **Feasibility:** [2,2,2]
  - **Metascientist without human:**
    - **Hypothesis:** To improve the structural efficiency of lattice materials, we propose a novel hypothesis that involves the design of a multi-layered lattice structure with a specific focus on a gradient-based transition between two distinct configurations: a gyroid-based TPMS and a diamond-based TPMS. The design will consist of three layers, each with a unique configuration to optimize mechanical properties. The top layer will utilize a gyroid TPMS structure, characterized by its high stiffness and minimal surface area, to provide initial load distribution and stress uniformity. The middle layer will transition into a diamond TPMS structure, which offers enhanced energy absorption and strength due to its interconnected nodal design. The bottom layer will revert to a gyroid TPMS, ensuring a balanced load transfer and structural integrity. Nodes within each unit cell will be connected using a continuous curvature approach to minimize stress concentrations and enhance load-bearing capacity. This hierarchical design strategy aims to achieve a synergistic effect, optimizing both stiffness and strength while maintaining a lightweight structure. The proposed hypothesis can be validated through experimental fabrication and

    mechanical testing, focusing on parameters such as compressive strength, stiffness, and energy absorption. This approach holds significant potential for advancing the design of lightweight, high-performance materials in applications ranging from aerospace to biomedical engineering.
    - **Reviewer Comment:** Lack of novelity, but the proposed structure design is very specific.
    - **Novelty:** [0,1,0]
    - **Feasibility:** [1,2,2]
  - **Metascientist with human:**
    - **Hypothesis:** In response to the question of improving the structural efficiency of lattice materials, this revised hypothesis proposes the development of a bio-inspired, hierarchical lattice structure that leverages the synergistic enhancement of mechanical properties. By exploring the intricate microstructural organization found in natural materials such as the nacreous layers of mollusk shells and the micro-architectures within coral skeletons, which exhibit remarkable mechanical efficiency through multi-scale architectures, this approach aims to integrate nano-sized features for local stiffness and strength, transitioning to larger structural elements for overall stability and load distribution. The hypothesis suggests that material gradation, akin to natural transitions between hard and soft regions, will promote stress distribution and energy absorption, thereby enhancing the structural efficiency of lattice materials. This innovative pathway, grounded in the meticulous analysis of diverse biological precedents, promises to significantly advance the field of mechanical metamaterials through experimental validation and computational modeling.
    - **Reviewer Comment:** Bioinspired strageties are quite common in research, but it is a highly feasible approach.
    - **Novelty:** [1,2,1]
    - **Feasibility:** [2,1,1]

- **Example 3**
  - **Topic:** improving damage tolerance
  - **Question:** One critical limitation to cellular ceramic materials are their brittleness and low damage tolerance. Can you propose some novel scientific hypotheses in how to improve the damage tolerance of lattice materials, which can be validated and are feasible to produce based on current manufacturing approaches?
  - **GPT-4o:**
    - **Hypothesis:** To address the inherent brittleness and low damage tolerance of cellular ceramic materials, we propose the development of a hierarchical lattice structure that integrates a combination of periodic and stochastic design elements. This approach leverages the mechanical advantages of both periodic and stochastic structures to enhance energy absorption and crack deflection capabilities. Specifically, we hypothesize that embedding a periodic lattice framework, such as a Kelvin or BCC structure, with stochastic elements like Voronoi foam, will create a synergistic effect that improves the overall toughness of the material. The periodic lattice provides a predictable load distribution and structural integrity, while the stochastic elements introduce randomness that can disrupt crack propagation pathways, thereby enhancing damage tolerance. This hybrid design can be feasibly manufactured using advanced additive manufacturing techniques, such as selective laser sintering or stereolithography, which allow for precise control over complex geometries at multiple scales. By optimizing the hierarchical arrangement and material composition, this novel lattice structure is expected to exhibit superior mechanical performance, making it a promising candidate for applications requiring high damage tolerance in ceramic materials.
    - **Reviewer Comment:** Structural radomness is a method proposed reletively recently, but it's not new. The usage of Kelvin or BCC lattices cannot grarantee high stiffness and strength, which impedes the feasibility of the hypothesis.

    - **Novelty:** [1,1,1]
    - **Feasibility:** [1,2,2]
  - **Metascientist without human:**
    - **Hypothesis:** To improve the damage tolerance of cellular ceramic materials, we propose the design of a novel lattice structure that employs a multi-layered approach, integrating a periodic Kelvin lattice at the core with a surrounding layer of stochastic Voronoi foam. The core Kelvin lattice, composed of truncated octahedra, ensures efficient load distribution and structural integrity, while the outer Voronoi foam layer introduces randomness to disrupt crack propagation pathways. This design leverages the mechanical stability of the Kelvin lattice, with its high strength-to-weight ratio, and the energy absorption capabilities of the stochastic layer. The nodes within the unit cell of the Kelvin lattice are connected via struts that are optimized for axial and bending loads, ensuring a balance between stiffness and flexibility. The hierarchical arrangement is further enhanced by varying the strut thickness and material composition across layers, allowing for tailored mechanical properties. This structure is expected to exhibit a Young's modulus of approximately 1.1e-3, a shear modulus of 8.5e-4, and a Poisson's ratio of 0.32, making it a promising candidate for applications requiring high damage tolerance. The proposed lattice can be feasibly manufactured using advanced additive manufacturing techniques, such as selective laser sintering, which allow for precise control over complex geometries and material distribution.
    - **Reviewer Comment:** Introducing structural radomness to enhance toughness is a method proposed reletively recently. The usage of Kelvin or BCC lattices cannot grarantee high stiffness and strength, which impedes the feasibility of the hypothesis. Additionally, the values of Young's modulus of approximately 1.1e-3, a shear modulus of 8.5e-4, and Poisson's ratio of 0.32 lack reasoning.
    - **Novelty:** [1,1,1]
    - **Feasibility:** [0,1,2]
  - **Metascientist with human:**
    - **Hypothesis:** To enhance the damage tolerance of ceramic lattice materials, this research proposes the development of a multi-step interlocking interface inspired by the sacrificial bonds found in bone. The key design principle involves creating a hierarchical interlocking mechanism within the lattice structure, consisting of primary, secondary, and tertiary interlocks. These interlocks are strategically designed to engage sequentially under increasing loads, providing multiple levels of energy dissipation and crack deflection. By mimicking the multi-level sacrificial bonding mechanism of bone, this approach aims to significantly improve the fracture toughness and damage tolerance of ceramic materials. The hypothesis will be validated through computational modeling and experimental testing, focusing on optimizing the geometry and material distribution to achieve maximum toughness without compromising structural integrity.
    - **Reviewer Comment:** multi-step interlocking interface inspired by the sacrificial bonds of bone is interesting.
    - **Novelty:** [2,2,2]
    - **Feasibility:** [2,1,2]

- **Example 4**
  - **Topic:** new auxetic metamaterials
  - **Question:** How can we innovate a new auxetic metamaterials that have negative Possion's ratio yet keep a high relative modulus? Please provide detailed design idea and highlight its potential advantages compared to other existing auxetic metamaterials.
  - **GPT-4o:**
    - **Hypothesis:** In response to the challenge of developing a novel auxetic metamaterial that exhibits a negative Poisson's ratio while maintaining a high relative modulus, we propose

the design and fabrication of a hierarchical re-entrant structure integrated with a stretch-dominated lattice framework. The motivation for this approach stems from the need to overcome the traditional trade-off between auxetic behavior and mechanical stiffness, which often limits the practical applications of auxetic materials. By employing a hierarchical design, we can leverage the benefits of multiple length scales to enhance mechanical properties. The re-entrant structure, known for its auxetic characteristics, will be strategically embedded within a stretch-dominated lattice, which is inherently capable of supporting high loads due to its efficient load distribution and connectivity. This combination is expected to synergistically enhance the overall mechanical performance, providing a metamaterial that not only exhibits a negative Poisson's ratio but also achieves a high relative modulus. Compared to existing auxetic metamaterials, this design offers the potential advantage of improved mechanical robustness and versatility, making it suitable for applications requiring both flexibility and strength, such as in advanced protective gear, biomedical devices, and adaptive architectural structures. The proposed metamaterial could thus represent a significant advancement in the field, offering a new paradigm for the design of multifunctional materials.
    * **Reviewer Comment:** Lack of novelity. Re-entrant structure and a stretch-dominated lattice framework does not simply add together. How to achive this is not explained.
    * **Novelty:** [0,1,1]
    * **Feasibility:** [0,2,2]
- **Metascientist without human:**
    * **Hypothesis:** To innovate a new auxetic metamaterial that exhibits a negative Poisson's ratio while maintaining a high relative modulus, we propose the design of a hierarchical re-entrant honeycomb structure integrated with a stretch-dominated lattice framework. This design aims to address the traditional trade-off between auxetic behavior and mechanical stiffness. The re-entrant honeycomb structure, characterized by its inverted angles, will be strategically embedded within a stretch-dominated lattice. The unit cell will consist of a central re-entrant honeycomb core surrounded by a network of axially aligned struts forming a stretch-dominated lattice. Each layer of the lattice will alternate between re-entrant and stretch-dominated configurations, with nodes connecting at the vertices of the re-entrant angles and the endpoints of the struts. This configuration allows for efficient load distribution and enhanced mechanical properties. The hierarchical design leverages multiple length scales to optimize the material's mechanical performance, achieving a negative Poisson's ratio while maintaining a high relative modulus. Compared to existing auxetic metamaterials, this design offers improved mechanical robustness and versatility, making it suitable for applications requiring both flexibility and strength, such as advanced protective gear, biomedical devices, and adaptive architectural structures.
    * **Reviewer Comment:** Lack of novelity.The proposed structure arrangement is very detailed but does not make sense.
    * **Novelty:** [0,1,2]
    * **Feasibility:** [0,2,2]
- **Metascientist with human:**
    * **Hypothesis:** In response to the challenge of developing auxetic metamaterials that exhibit a negative Poisson's ratio while maintaining a high relative modulus, we propose a novel approach that eschews the traditional reliance on reentrant joints and folding mechanisms, which are often associated with reduced mechanical efficiency and increased manufacturing complexity. Instead, our design leverages a plate-based structure that integrates strategic perforated patterns with material anisotropy and gradient material properties. By utilizing tessellated perforations, such as hexagonal or triangular grids, and capitalizing on the directional properties of advanced composite materials like fiber-reinforced polymers, the structure is engineered to expand laterally under tensile loads, thereby achieving the desired

  auxetic behavior. The incorporation of a gradient in material properties further optimizes stress distribution, enhancing the auxetic response while maintaining structural integrity. This innovative design not only addresses the traditional trade-off between auxeticity and stiffness but also ensures high mechanical efficiency, scalability, and manufacturability using conventional techniques. Moreover, it offers significant versatility, allowing for customization to meet specific application requirements across diverse fields such as aerospace, automotive, and consumer products. By focusing on these advanced design principles, our approach presents a promising pathway for advancing the capabilities and applications of auxetic metamaterials.
    - **Reviewer Comment:** The hypotheis address the critial constrain that reentrant and folding are often necessary for achieving auxetic properties but reduces mechanical efficiency and proposed an interesing differnet approch.
    - **Novelty:** [1,2,2]
    - **Feasibility:** [2,1,1]

- **Example 5**
  - **Topic:** overcoming mechanical tradeoff between stiffness and toughness
  - **Question:** Mechanical tradeoff between strength and toughness is a long lasting question in materials design, can you propose some novel, testable ideas to overcome this tradeoff by designing lattice metamaterails?
  - **GPT-4o:**
    - **Hypothesis:** In addressing the longstanding mechanical tradeoff between strength and toughness in materials design, we propose the development of a novel lattice metamaterial that leverages a hierarchical, open-cell structure with a focus on periodic, stretch-dominated configurations. Specifically, we hypothesize that a combination of octet and diamond lattice structures, arranged in a hierarchical manner, can be engineered to achieve an optimal balance between strength and toughness. The octet lattice, known for its high strength due to its stretch-dominated nature, will provide the necessary structural integrity, while the diamond lattice, with its inherent ability to distribute stress and absorb energy, will enhance toughness. By integrating these two lattice types at different hierarchical levels, we anticipate that the resulting metamaterial will exhibit superior mechanical properties, overcoming the traditional tradeoff. This approach is motivated by the potential to exploit the unique mechanical interactions at multiple scales, thereby enabling the design of materials that are both strong and tough. The proposed hypothesis will be tested through computational modeling and experimental validation, focusing on the mechanical performance under various loading conditions to confirm the synergistic effects of the hierarchical lattice design.
    - **Reviewer Comment:** Known stragety. How to improve toughness through controlling "mechanical interactions at multiple scales" is not clear.
    - **Novelty:** [0,1,0.5]
    - **Feasibility:** [1,2,2]
  - **Metascientist without human:**
    - **Hypothesis:** To address the mechanical tradeoff between strength and toughness in materials design, we propose a novel lattice metamaterial that utilizes a hierarchical, open-cell structure with a focus on periodic, stretch-dominated configurations. Specifically, we hypothesize that a lattice structure composed of alternating layers of octet and diamond configurations, arranged in a hierarchical manner, can achieve an optimal balance between strength and toughness. The design involves a unit cell where the octet lattice forms the core, providing high strength and structural integrity through its stretch-dominated nature, while the diamond lattice forms the outer shell, enhancing toughness by distributing stress and absorbing energy. The nodes in the unit cell are connected through a series of tetrahedral and

    diamond-like struts, ensuring efficient load transfer and energy dissipation. The hierarchical arrangement is designed to exploit mechanical interactions at multiple scales, with the octet core having a relative density of 0.2 and the diamond shell a relative density of 0.15. This configuration is expected to yield a Young's modulus of approximately 1.1e-3 GPa, a shear modulus of 8.5e-4 GPa, and a Poisson's ratio of 0.32. The proposed hypothesis will be tested through computational modeling and experimental validation, focusing on the mechanical performance under various loading conditions to confirm the synergistic effects of the hierarchical lattice design.
    - **Reviewer Comment:** The core-shell structure in lattice application is interesting. While novel idea is involved, the realization of the idea is problematic - the detailed design does not make sense.
    - **Novelty:** [2,1,1]
    - **Feasibility:** [0,1,1]
  - **Metascientist with human:**
    - **Hypothesis:** In addressing the persistent challenge of balancing strength and toughness in materials design, this research proposes the development of a novel lattice metamaterial inspired by the multi-step interlocking mechanisms observed in natural systems, such as the sacrificial bonds in bone. The hypothesis posits that by incorporating a hierarchical interlocking interface within the lattice structure, consisting of primary, secondary, and tertiary interlocks, it is possible to achieve enhanced energy dissipation and crack deflection, thereby overcoming the traditional tradeoff between strength and toughness. This design strategy involves the sequential engagement of interlocks under increasing loads, which provides multiple levels of energy absorption and crack arrest, akin to the multi-level sacrificial bonding mechanism found in biological materials. The proposed metamaterial will be fabricated using advanced additive manufacturing techniques, allowing for precise control over the hierarchical interlocking features. Validation of this hypothesis will be conducted through a combination of computational modeling and experimental testing, focusing on optimizing the geometry and material distribution to maximize toughness while maintaining structural integrity. This research aims to advance the field of mechanical metamaterials by introducing a biomimetic approach that offers a promising solution to the longstanding challenge of designing materials that do not compromise on either strength or toughness.
    - **Novelty:** [2,1.5,2]
    - **Feasibility:** [2,1,2]

- **Example 6**
  - **Topic:** adjustable materials properties
  - **Question:** Lattice materials can be designed to have a wide property space by changing their structure parameters. How to design a single lattice material and its property can be widely adjusted?
  - **GPT-4o:**
    - **Hypothesis:** In response to the challenge of designing a single lattice material with widely adjustable properties, we propose the development of a tunable lattice structure utilizing a hierarchical approach combined with a periodic open-cell design, specifically focusing on the octet lattice configuration. The motivation for this approach stems from the inherent versatility of hierarchical structures, which allow for multi-scale property tuning, and the octet lattice's well-documented mechanical efficiency and isotropic behavior. By integrating hierarchical design principles, we can introduce multiple levels of structural organization within the octet lattice, enabling the modulation of mechanical properties such as stiffness, strength, and toughness. This multi-scale design strategy will facilitate the fine-tuning of the lattice's mechanical response through the adjustment of parameters at different hierarchical

    levels, such as cell size, strut thickness, and connectivity. Additionally, the periodic nature of the octet lattice ensures uniformity and predictability in mechanical performance, which is crucial for applications requiring precise control over material properties. This approach not only broadens the property space of the lattice material but also enhances its adaptability for various engineering applications, ranging from lightweight structural components to impact-resistant materials.
  - **Novelty:** [0,1,0.5]
  - **Feasibility:** [0,2,2]
- **Metascientist without human:**
  - **Hypothesis:** To address the challenge of designing a single lattice material with widely adjustable properties, we propose a novel lattice structure that leverages a periodic open-cell design with a focus on the octet lattice configuration. This design will incorporate a multi-layered approach, where each layer consists of a distinct arrangement of tetrahedral and octahedral units. The nodes within each unit cell will be connected through a network of struts with varying thicknesses, allowing for precise control over the mechanical properties. The hierarchical design will be implemented by introducing multiple scales of structural organization, enabling the modulation of properties such as stiffness, strength, and toughness. Specifically, the lattice will be constructed with a base layer of octahedral units, providing isotropic mechanical behavior, while subsequent layers will incorporate tetrahedral units to enhance directional stiffness. The connectivity between nodes will be optimized to ensure uniform stress distribution and minimize localized buckling. By adjusting parameters such as cell size, strut thickness, and node connectivity, the lattice can achieve a wide range of mechanical properties, making it suitable for diverse engineering applications. This approach not only broadens the property space of the lattice material but also enhances its adaptability for applications requiring precise control over material properties.
  - **Novelty:** [0,1,0.5]
  - **Feasibility:** [0,2,1]
- **Metascientist with human:**
  - **Hypothesis:** We propose the development of a novel lattice material that exploits the controlled buckling of its structural elements to achieve a wide range of adjustable mechanical properties. The key novelty of this approach lies in the precise control of the onset of buckling, allowing the material to transition between high-stiffness (non-buckled) and low-stiffness (buckled) states. By designing the lattice with elements that can be selectively triggered to buckle, the material can dynamically adjust its stiffness in response to external loads or environmental conditions. This approach leverages the significant difference in mechanical properties between the buckled and non-buckled states to provide a simple yet effective means of tunability. Potential mechanisms for controlling buckling include the use of pre-stressed elements that can be selectively released, variable cross-sections that adjust the critical buckling load, and localized thermal or electromagnetic activation to induce targeted buckling. This research aims to explore these mechanisms to develop a versatile lattice material with applications in adaptive structures, impact mitigation, and deployable systems, where tunable stiffness is advantageous. By harnessing the inherent geometric nonlinearity of buckling, this approach offers a promising avenue for creating advanced metamaterials with customizable mechanical properties, while maintaining energy efficiency and design simplicity.
  - **Reviewer Comment:** Controlling when buckling happens to adjust stiffness is both interesting and feasible, as a material in its buckled state can be significantly softer than it is in non-buckled state.
  - **Novelty:** [1,2,1]
  - **Feasibility:** [2,1.5,2]

- **Example 7**
  - **Topic:** bioinspired metamaterials
  - **Question:** Can you provide a few examples of biological metamaterials with amazing materials properties, based on which further design bioinspired metamaterials?
  - **GPT-4o:**
    - **Hypothesis:** Biological metamaterials, such as the nacre of mollusk shells, the lightweight yet strong structure of bird bones, and the flexible yet resilient composition of spider silk, offer remarkable insights into the design of bioinspired mechanical metamaterials. Nacre, with its hierarchical structure of aragonite platelets and organic matrix, exhibits exceptional toughness and strength, serving as a model for creating layered composite metamaterials with enhanced fracture resistance. Bird bones, characterized by their hollow, lattice-like structure, provide inspiration for designing lightweight, high-strength metamaterials using periodic lattice configurations such as the octet or Kelvin structures, which can optimize load distribution while minimizing material usage. Spider silk, known for its extraordinary tensile strength and elasticity, suggests the potential for developing metamaterials with tunable mechanical properties through the incorporation of hierarchical and disorder-based design principles. By emulating these natural structures, it is hypothesized that novel bioinspired metamaterials can be engineered to achieve a balance of strength, toughness, and lightweight characteristics, offering significant advancements in applications ranging from aerospace to biomedical devices. This approach not only leverages the inherent advantages of biological systems but also paves the way for sustainable and efficient material design.
    - **Novelty:** [0,1,1]
    - **Feasibility:** [2,1,2]
  - **Metascientist without human:**
    - **Hypothesis:** To design bioinspired mechanical metamaterials with enhanced mechanical properties, we propose a lattice structure inspired by the hierarchical organization of nacre and the lightweight architecture of bird bones. The proposed design consists of a multi-layered composite structure where each layer mimics the brick-and-mortar arrangement of nacre, with aragonite-like platelets interspersed within an organic matrix analog. This configuration is expected to enhance fracture resistance and toughness. The unit cell of the lattice is designed as a hollow, periodic structure, similar to bird bones, to optimize the strength-to-weight ratio. Each node within the unit cell is connected through a truss-like network, ensuring efficient load distribution and minimizing material usage. The hierarchical design strategy incorporates varying thicknesses of the internal surfaces to transition from shear-compliant to compression-compliant behaviors, inspired by the lipidic cubic phases. The expected mechanical properties of this lattice are tailored to achieve a Young's modulus of approximately 1.1e-3, a Shear modulus of 8.5e-4, and a Poisson's ratio of 0.32, aligning with the desired balance of strength, toughness, and lightweight characteristics. This approach leverages the inherent advantages of biological systems, paving the way for sustainable and efficient material design in applications ranging from aerospace to biomedical devices.
    - **Novelty:** [0,1,1]
    - **Feasibility:** [1,1,2]
  - **Metascientist with human:**
    - **Hypothesis:** In the quest to develop bioinspired metamaterials with superior thermal management and ice-resistant properties, it is hypothesized that integrating the thermal insulating characteristics of polar bear fur with the ice-resistant capabilities of antifreeze proteins found in fish can lead to the creation of a novel metamaterial. This metamaterial will feature a hierarchical porous lattice structure that effectively traps air for insulation, akin to the hollow tubular hairs of polar bear fur, while its surface will be functionalized with

    antifreeze protein-mimetic molecules found in fish to inhibit ice formation. The resulting material is expected to be lightweight, durable, and adaptable to extreme cold environments, making it highly suitable for applications in clothing, aerospace, marine, and building materials. By leveraging the unique properties of these biological inspirations, this research aims to address the challenges of operating in cold climates, enhancing performance and safety, and demonstrating the potential of bioinspired design in advancing the field of mechanical metamaterials.

    - **Novelty:** [2,2,2]
    - **Feasibility:** [2,1,2]

- **Example 8**
  - **Topic:** novel lattice materials for biomedical applications
  - **Question:** Our goal is to develop new ways of applying lattice materials for the broad scope of biomedical application. We want the novel concept to have high impact to human benefit. Can you generated some novel research ideas and some concise reasoning behind these ideas?
  - **GPT-4o:**
    - **Hypothesis:** In the pursuit of advancing biomedical applications through the innovative use of lattice materials, we propose the development of a bio-inspired, open-cell lattice structure with a focus on the periodic Kagome configuration. This structure is hypothesized to exhibit exceptional mechanical properties, such as high strength-to-weight ratio and enhanced energy absorption capabilities, which are critical for applications in bone scaffolding and tissue engineering. The Kagome lattice, characterized by its unique geometric arrangement, offers a promising platform for mimicking the hierarchical and anisotropic properties of natural bone, thereby facilitating improved integration and load distribution in implantable devices. Furthermore, by incorporating tunable properties such as modulus and strength through controlled truss waviness and connectivity, the proposed lattice can be tailored to match the mechanical behavior of various biological tissues. This adaptability not only enhances the biocompatibility and functionality of the implants but also opens avenues for personalized medicine, where patient-specific lattice structures can be designed to optimize healing and recovery. The successful implementation of this concept could significantly impact human health by improving the efficacy and longevity of biomedical implants, ultimately leading to better patient outcomes and quality of life.
    - **Novelty:** [1,1.5,1]
    - **Feasibility:** [2,1.5,1]
  - **Metascientist without human:**
    - **Hypothesis:** To advance biomedical applications through the innovative use of lattice materials, we propose the development of a bio-inspired, open-cell lattice structure with a focus on a periodic, multi-layered configuration. This structure is designed to exhibit exceptional mechanical properties, such as a high strength-to-weight ratio and enhanced energy absorption capabilities, which are critical for applications in bone scaffolding and tissue engineering. The proposed lattice consists of a three-layered design, where each layer is composed of a distinct geometric arrangement to optimize mechanical performance. The top layer features a hexagonal pattern to maximize surface area and facilitate nutrient flow, the middle layer employs a triangular configuration for enhanced load distribution, and the bottom layer utilizes a square grid to provide structural stability. Nodes within the unit cell are connected using a hierarchical design strategy, where primary nodes are reinforced with secondary trusses to enhance stiffness and resilience. By incorporating tunable properties such as modulus and strength through controlled truss thickness and connectivity, the proposed lattice can be tailored to match the mechanical behavior of various biological tissues. This adaptability not only enhances the biocompatibility and functionality of the implants but also opens avenues for personalized medicine, where patient-specific lattice

    structures can be designed to optimize healing and recovery. The successful implementation of this concept could significantly impact human health by improving the efficacy and longevity of biomedical implants, ultimately leading to better patient outcomes and quality of life.
    - **Novelty:** [1,1.5,1]
    - **Feasibility:** [2,1.5,1]
  - **Metascientist with human:**
    - **Hypothesis:** In the quest to advancing neural interface technology, we propose the development of a multifunctional neural interface that synergistically integrates hierarchical lattice designs, embedded sensors, and flexible materials. The hierarchical lattice structure is engineered to mimic the natural extracellular matrix, thereby enhancing cell adhesion, proliferation, and synapse formation, which are critical for stable and long-lasting neural connections. Embedded sensors within the lattice will facilitate real-time monitoring of neural activity and tissue health, providing continuous feedback that is crucial for personalized treatment and early detection of complications. The use of flexible, biocompatible materials aims to minimize mechanical mismatch and immune response, addressing significant challenges in neural interface development such as biocompatibility, mechanical stability, and long-term durability. This innovative approach is designed to improve the integration and functionality of neural interfaces, ultimately leading to enhanced patient outcomes in neuroprosthetics and brain-machine interface applications. By addressing these critical challenges, this research endeavors to contribute significantly to the advancement of neural engineering and regenerative medicine, offering new possibilities for individuals with neurological disorders.
    - **Novelty:** [2,1.5,2]
    - **Feasibility:** [2,1,1]

- **Example 9**
  - **Topic:** novel lattice materials for art and design
  - **Question:** How can we innovate a new lattice materials concepts for visual arts and design? Please provide detailed structure design idea and highlight its novelty.
  - **GPT-4o:**
    - **Hypothesis:** In response to the question of innovating new lattice material concepts for visual arts and design, we propose the development of a novel lattice structure based on the Kagome configuration, enhanced with a hierarchical design approach. The Kagome lattice, known for its unique geometric arrangement of interlaced triangles, offers an aesthetically pleasing pattern that can be leveraged for artistic applications. By integrating a hierarchical design, where smaller Kagome units are nested within larger ones, we can achieve a multi-scale visual complexity that enhances the visual appeal and structural integrity of the material. This hierarchical Kagome lattice not only provides a captivating visual experience but also introduces a new dimension of tunable mechanical properties, such as enhanced stiffness and strength, which are crucial for practical applications in design and architecture. The novelty of this approach lies in its ability to merge the artistic elegance of the Kagome pattern with the functional benefits of hierarchical structuring, offering a versatile material that can be tailored for both aesthetic and structural purposes in visual arts and design. This innovative concept has the potential to redefine the boundaries of material usage in creative industries, providing artists and designers with a new tool to explore form and function in their work.
    - **Novelty:** [0,1,1]
    - **Feasibility:** [2,1,2]
  - **Metascientist without human:**

        - **Hypothesis:** To innovate new lattice material concepts for visual arts and design, we propose the development of a novel lattice structure based on a modified Kagome configuration, enhanced with a multi-layered design approach. The Kagome lattice, characterized by its geometric arrangement of interlaced triangles, is aesthetically appealing and offers unique mechanical properties. Our approach involves a three-layered structure where each layer consists of a Kagome lattice with varying node connectivity and strut thickness. The first layer features a standard Kagome pattern with uniform node connections, providing a base level of structural integrity. The second layer introduces a variation in node connectivity, where every alternate node is connected to an additional strut, enhancing the stiffness and visual complexity. The third layer incorporates a gradient in strut thickness, transitioning from thicker struts at the center to thinner ones at the edges, optimizing the material for both strength and light transmission. This design not only enhances the visual appeal but also allows for tunable mechanical properties, such as increased stiffness and strength, which are crucial for practical applications in design and architecture. The novelty of this approach lies in its ability to merge the artistic elegance of the Kagome pattern with the functional benefits of a multi-layered structuring, offering a versatile material that can be tailored for both aesthetic and structural purposes in visual arts and design. This innovative concept has the potential to redefine the boundaries of material usage in creative industries, providing artists and designers with a new tool to explore form and function in their work.
        - **Novelty:** [0,1,0.5]
        - **Feasibility:** [2,1,1]
    - **Metascientist with human:**
        - **Hypothesis:** In response to the growing intersection of visual arts and material science, we propose the development of a Dynamic Morphing Lattice (DML) that leverages nature-inspired patterns and smart materials to create a responsive and interactive medium for visual arts and design. The DML is designed to exhibit dynamic shape transformations in response to environmental stimuli, such as temperature and humidity changes, by integrating materials like shape-memory alloys and polymers. This approach not only enhances the aesthetic appeal of art installations but also introduces a functional aspect, allowing artworks to evolve and engage viewers through environmental interaction. The novelty of this concept lies in its ability to combine the beauty of natural patterns with the mechanical versatility of advanced materials, offering a sustainable and innovative platform for creative expression. By employing advanced fabrication techniques, such as additive manufacturing, the DML can be customized in terms of geometry and material composition, providing artists and designers with a versatile tool for exploring new artistic possibilities.
        - **Novelty:** [1,2,2]
        - **Feasibility:** [2,1,2]

- **Example 10**
    - **Topic:** novel mechancial metamaterials beyond the elastic regime
    - **Question:** Negative index materials are typically based on the parameters of materials in the elastic regime. Can we generate metamaterials based on the nonlinear properties of materials?
    - **GPT-4o:**
        - **Hypothesis:** In response to the question of whether metamaterials can be generated based on the nonlinear properties of materials, we propose the development of a novel class of mechanical metamaterials that exploit the nonlinear elastic behavior of constituent materials to achieve negative index properties. Traditional negative index materials have predominantly relied on linear elastic parameters, limiting their functional range and adaptability. By harnessing the nonlinear characteristics, such as strain-stiffening or softening, we can design metamaterials that exhibit tunable negative index properties under varying mechanical loads. This approach involves the strategic design of open-cell periodic structures, specifically

focusing on lattice configurations such as the octet or diamond, which are known for their ability to accommodate large deformations. By incorporating materials with inherent nonlinear elastic responses, these structures can be engineered to exhibit negative stiffness or negative Poisson's ratio under specific loading conditions, thereby expanding the operational bandwidth and functionality of negative index metamaterials. This hypothesis not only challenges the conventional reliance on linear properties but also opens new avenues for the design of adaptive and multifunctional metamaterials, with potential applications in advanced vibration isolation, impact mitigation, and acoustic cloaking technologies.
    - **Novelty:** [1,1,1]
    - **Feasibility:** [1,1,2]
- **Metascientist without human:**
    - **Hypothesis:** To address the question of whether metamaterials can be generated based on the nonlinear properties of materials, we propose the design of a novel mechanical metamaterial that leverages the nonlinear elastic behavior of its constituent materials to achieve negative index properties. Traditional approaches have predominantly relied on linear elastic parameters, which limit the functional range and adaptability of these materials. Our approach involves the strategic design of a multi-layered lattice structure, where each layer consists of a diamond lattice configuration. The diamond lattice is chosen for its ability to balance strength and flexibility, allowing for large elastic deformations. Each unit cell within the lattice is composed of tetrahedral units, interconnected at nodes to form a continuous network. The nodes are designed to allow rotational freedom, enhancing the structure's ability to accommodate nonlinear deformations. By incorporating materials with inherent nonlinear elastic responses, such as strain-stiffening or softening, the lattice can be engineered to exhibit negative stiffness or negative Poisson's ratio under specific loading conditions. This design not only challenges the conventional reliance on linear properties but also opens new avenues for the creation of adaptive and multifunctional metamaterials, with potential applications in advanced vibration isolation, impact mitigation, and acoustic cloaking technologies.
    - **Novelty:** [1,1,1]
    - **Feasibility:** [1,1,1]
- **Metascientist with human:**
    - **Hypothesis:** In response to the research question of whether metamaterials can be generated based on the nonlinear properties of materials, we propose the development of a novel class of mechanical metamaterials that leverage hysteresis as a nonlinear mechanism to achieve tunable negative index properties. Traditional approaches to negative index materials have predominantly focused on linear elastic parameters, thereby constraining their adaptability and functional range. By exploiting hysteresis, which introduces path-dependent behavior and memory effects, we can design metamaterials that exhibit dynamically adjustable negative indices in response to varying mechanical loads. This approach involves engineering periodic lattice structures composed of materials with pronounced hysteretic behavior, enabling controlled hysteretic cycles that allow for reversible transitions between different mechanical states. The metamaterial can thus "remember" previous states and adjust its mechanical response accordingly, providing a tunable negative index modulated by the history of applied stress or strain. This innovative use of hysteresis not only broadens the operational bandwidth of negative index metamaterials but also introduces a new paradigm in the design of adaptive and responsive material systems. Such advancements hold significant potential for applications in wave manipulation, vibration control, and advanced sensing technologies, where the ability to adapt to changing conditions and retain memory of past interactions is highly advantageous.
    - **Novelty:** [2,2,2]
    - **Feasibility:** [1,1,1]

- **Example 11**
  - **Topic:** novel multifunctional lattice metamaterials
  - **Question:** Please develop a novel concept of multifunctional metamaterial, illustrate the principles and the potential applications.
  - **GPT-4o:**
    - **Hypothesis:** In response to the question of integrating mechanical metamaterials with electromagnetic metamaterials, we propose the development of a novel class of multifunctional metamaterials that leverage the unique properties of both domains to achieve unprecedented control over mechanical and electromagnetic responses. The motivation for this research stems from the growing demand for materials that can simultaneously manage mechanical loads and electromagnetic fields, which is critical in applications such as advanced sensors, actuators, and energy harvesting devices. Our approach involves the design of a periodic open-cell lattice structure, specifically utilizing a TPMS (Triply Periodic Minimal Surface) configuration, which inherently provides a high surface area-to-volume ratio and mechanical robustness. This structure will be embedded with conductive pathways and magnetic inclusions to facilitate electromagnetic interactions. By exploiting the tunable modulus and strength properties of the mechanical lattice, alongside the negative permittivity and permeability characteristics of the electromagnetic components, we aim to create a metamaterial that exhibits both mechanical resilience and electromagnetic tunability. This integration is expected to result in a synergistic enhancement of material performance, enabling the development of devices that can adapt to dynamic environments and multifunctional requirements.
    - **Novelty:** [1,2,1]
    - **Feasibility:** [2,1,2]
  - **Metascientist without human:**
    - **Hypothesis:** To address the integration of mechanical metamaterials with electromagnetic metamaterials, we propose the design of a multifunctional metamaterial that combines the mechanical robustness of a Triply Periodic Minimal Surface (TPMS) lattice with embedded electromagnetic functionalities. The TPMS structure will be configured using a gyroid surface, characterized by its continuous, non-self-intersecting geometry, which provides a high surface area-to-volume ratio and inherent mechanical strength. Each unit cell will consist of a gyroid lattice with a node connectivity that ensures isotropic mechanical properties, while maintaining a minimal surface configuration to optimize material usage. Conductive pathways will be strategically embedded within the lattice, following the gyroid's curvature, to facilitate electromagnetic interactions. These pathways will be composed of a high-conductivity material, such as silver, to ensure efficient electromagnetic response. Magnetic inclusions, in the form of nanoscale ferromagnetic particles, will be dispersed within the lattice to enhance electromagnetic tunability. The mechanical properties of the lattice will be fine-tuned to achieve a Young's modulus of approximately 1.1e-3 GPa, a Shear modulus of 8.5e-4 GPa, and a Poisson's ratio of 0.32, ensuring a balance between mechanical resilience and electromagnetic functionality. This design aims to create a metamaterial capable of adapting to dynamic environments, with potential applications in advanced sensors, actuators, and energy harvesting devices.
    - **Novelty:** [1,2,1]
    - **Feasibility:** [1,1,2]
  - **Metascientist with human:**
    - **Hypothesis:** Integrating multifunctional metamaterials into clothing and exoskeletons will enhance human capabilities and comfort by providing adaptive support, dynamic thermal regulation, and impact protection. These metamaterials, featuring hierarchical structures and programmable properties, will enable personalized fit, real-time health monitoring,

and environmental responsiveness. This approach will lead to advanced wearable systems suitable for applications in healthcare, sports, military, and occupational safety.

- **Novelty:** [2,1,1.5]
- **Feasibility:** [1,1,2]