A Comprehensive Survey of Scientific Large Language Models and Their Applications in Scientific Discovery

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Abstract

In many scientific fields, large language models (LLMs) have revolutionized the way text and other modalities of data (*e.g.,* molecules and proteins) are handled, achieving superior performance in various applications and augmenting the scientific discovery process. Nevertheless, previous surveys on scientific LLMs often concentrate on one or two fields or a single modality. In this paper, we aim to provide a more holistic view of the research landscape by unveiling cross-field and cross-modal connections between scientific LLMs regarding their architectures and pre-training techniques. To this end, we comprehensively survey over 260 scientific LLMs, discuss their commonalities and differences, as well as summarize pre-training datasets and evaluation tasks for each field and modality. Moreover, we investigate how LLMs have been deployed to benefit scientific discovery. Resources related to this survey are available at `https://github.com/yuzhimanhua/Awesome-Scientific-Language-Models`.

1 Introduction

The emergence of large language models (LLMs) (Zhao et al., 2023c) brings a new paradigm to natural language processing (NLP) by replacing specialized models designed for each task with unified models that are reasonably effective for a wide spectrum of problems. In the scientific domain, such a paradigm not only reshapes people's strategies to handle tasks related to natural language (*e.g.,* scientific papers, medical records, and climate reports) but also inspires analogous ideas to deal with other types of data (*e.g.,* molecules, proteins, tables, and metadata). In addition to understanding existing scientific data, LLMs have shown their potential to accelerate scientific discovery (Wang et al., 2023c; Zhang et al., 2023e; Wang et al., 2024d) through generation, planning, *etc.*

Given the broad and profound impact of LLMs in various scientific fields across diverse modalities, it becomes necessary to comprehensively review related work in this direction. However, existing scientific LLM surveys typically focus on either one or two fields (*e.g.,* biomedicine (Wang et al., 2023a; He et al., 2024b; Pei et al., 2024; Zhang et al., 2024d) and chemistry (Xia et al., 2023; Pei et al., 2024; Zhang et al., 2024d)) or one modality (*e.g.,* text (Ho et al., 2024)) only. In fact, if we take a holistic view of the research landscape, we can observe similar and interrelated techniques used to develop LLMs for different fields and modalities.

Figure 1 depicts three major types of scientific LLM pre-training strategies (*i.e.,* COLUMNS 1 to 3), for each of which we give 4 examples (*i.e.,* TYPES A to D). In COLUMN 1, following BERT (Devlin et al., 2019) and RoBERTa (Liu et al., 2019), existing studies use masked language modeling (MLM) to pre-train encoder language models. Here, the input can be naturally sequential (*e.g.,* papers in each field; protein, DNA, and RNA sequences in the FASTA format (Lipman and Pearson, 1985)) or artificially linearized (*e.g.,* molecules in the SMILES format (Weininger, 1988); sequences of venue, author, and reference nodes in citation graphs). In COLUMN 2, inspired by GPT (Brown et al., 2020) and LLaMA (Touvron et al., 2023a), previous studies adopt next token prediction to pre-train (encoder-)decoder language models, some of which further adopt instruction tuning and preference optimization (Ouyang et al., 2022). Other than plain text input (*e.g.,* question-answer pairs from knowledge bases or exams), we see more ways to sequentialize complex scientific data, such as flattening table cells and using particle coordinates to describe crystals. Even for images, there are studies in both mathematics (Gao et al., 2023) and biomedicine (Li et al., 2023a) that exploit a vision encoder to project an image onto several visual tokens and prepend them to text tokens as linearized LLM input. In COLUMN 3,

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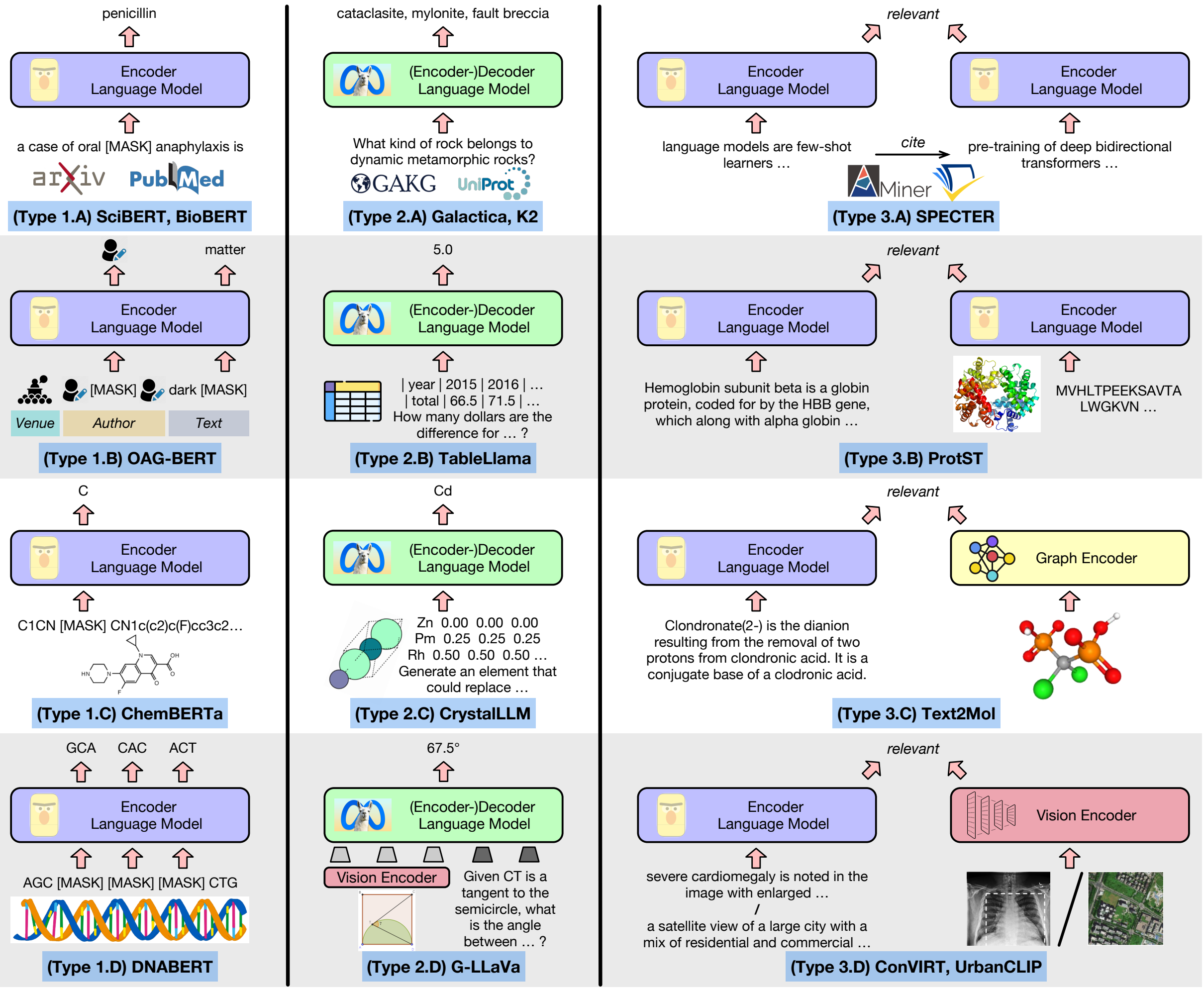
penicillin
Encoder Language Model
a case of oral [MASK] anaphylaxis is
arXiv
PubMed
(Type 1.A) SciBERT, BioBERT
cataclasite, mylonite, fault breccia
(Encoder-)Decoder Language Model
What kind of rock belongs to dynamic metamorphic rocks?
GAKG
UniProt
(Type 2.A) Galactica, K2
relevant
Encoder Language Model
Encoder Language Model
language models are few-shot learners …
cite
pre-training of deep bidirectional transformers …
AMiner
(Type 3.A) SPECTER
matter
Encoder Language Model
[MASK]
dark [MASK]
Venue
Author
Text
(Type 1.B) OAG-BERT
5.0
(Encoder-)Decoder Language Model
| year | 2015 | 2016 | …
| total | 66.5 | 71.5 | …
How many dollars are the difference for … ?
(Type 2.B) TableLlama
relevant
Encoder Language Model
Encoder Language Model
Hemoglobin subunit beta is a globin protein, coded for by the HBB gene, which along with alpha globin …
MVHLTPEEKSAVTA LWGKVN …
(Type 3.B) ProtST
C
Encoder Language Model
C1CN [MASK] CN1c(c2)c(F)cc3c2…
(Type 1.C) ChemBERTa
Cd
(Encoder-)Decoder Language Model
Zn 0.00 0.00 0.00
Pm 0.25 0.25 0.25
Rh 0.50 0.50 0.50 …
Generate an element that could replace …
(Type 2.C) CrystalLLM
relevant
Encoder Language Model
Graph Encoder
Clondronate(2-) is the dianion resulting from the removal of two protons from clondronic acid. It is a conjugate base of a clodronic acid.
(Type 3.C) Text2Mol
GCA
CAC
ACT
Encoder Language Model
AGC [MASK] [MASK] [MASK] CTG
(Type 1.D) DNABERT
67.5°
(Encoder-)Decoder Language Model
Vision Encoder
Given CT is a tangent to the semicircle, what is the angle between … ?
(Type 2.D) G-LLaVa
relevant
Encoder Language Model
Vision Encoder
severe cardiomegaly is noted in the image with enlarged …
/
a satellite view of a large city with a mix of residential and commercial …
(Type 3.D) ConVIRT, UrbanCLIP

Figure 1: Three major types of scientific LLM pre-training techniques. (**Column 1**): Pre-training encoder LLMs with sequentialized scientific data (*e.g.,* text, academic graphs, molecules, biological sequences) via masked language modeling. (**Column 2**): Pre-training (encoder-)decoder LLMs with sequentialized scientific data (*e.g.,* text, tables, crystals, images) via next token prediction (possibly with instruction tuning). (**Column 3**): Mapping text and relevant sequences/graphs/images closer in the latent space via contrastive learning.

following DPR (Karpukhin et al., 2020) and CLIP (Radford et al., 2021), two encoders are pre-trained to map relevant data pairs closer in the latent space via contrastive learning. When both modalities are sequential (*e.g.,* text-text or text-protein), the model is built upon two LLM encoders. When we prefer to keep the non-sequential nature of one modality (*e.g.,* molecular graphs (Edwards et al., 2021), chest X-rays (Zhang et al., 2022), and aerial views (Yan et al., 2024)), the corresponding graph or image encoder can be employed. To summarize, a cross-field, cross-modal survey will more accurately draw the connections between different scientific LLMs, demonstrate their commonalities, and potentially guide their future designs.

Contributions. In this paper, motivated by the discussions above, we systematically survey over 260 scientific LLMs encompassing various fields (*e.g.,* general science, mathematics, physics, chemistry, materials science, biology, medicine, and geoscience), modalities (*e.g.,* language, graph, vision, table, molecule, protein, genome, and climate time series), and sizes (from ∼100M to ∼100B parameters). For each field/modality, we investigate commonly adopted pre-training datasets, model architectures, and evaluation tasks of scientific LLMs. Following our motivation, when we discuss model architectures in detail, we link them back to Figure 1 to build cross-field cross-modal connections. Moreover, we provide a structured summary of these scientific LLMs in Table A1-Table A6 (Appendix A). Furthermore, for different fields, we introduce how LLMs have been deployed to benefit science by augmenting different aspects and stages of the scientific discovery process, such as hypothesis generation, theorem proving, experiment design, drug discovery, and weather forecasting.

2 LLMs in General Science (Table A1)

2.1 Language

The most commonly used pre-training corpora for scientific LLMs are research papers from bibliographic databases, such as AMiner (Tang et al., 2008), Microsoft Academic Graph (MAG) (Sinha et al., 2015), and Semantic Scholar (Ammar et al., 2018). Some of these sources (*e.g.,* S2ORC (Lo et al., 2020)) contain full-text information of papers, while the others have titles and abstracts only.

The evolution of scientific LLMs bears similarity to that of general-domain LLMs. Specifically, pioneering models utilize paper text in a self-supervised manner during pre-training, aiming to acquire scientific knowledge from large-scale unlabeled corpora. For example, masked language modeling (MLM) is the default pre-training task for scientific LLMs with a BERT backbone (TYPE 1.A in Figure 1, *e.g.,* SciBERT (Beltagy et al., 2019)); next token prediction is widely used for GPT-based scientific LLMs (TYPE 2.A in Figure 1, *e.g.,* SciGPT (Luu et al., 2021)). More recently, inspired by the fact that LLMs can be trained to follow natural language instructions (Wei et al., 2022a; Ouyang et al., 2022), researchers have put more effort into tuning LLMs with instructions to solve complex scientific problems (TYPE 2.A, *e.g.,* Galactica (Taylor et al., 2022) and SciGLM (Zhang et al., 2024a)). The instruction tuning data are often derived from datasets for downstream tasks, such as exam question answering (Welbl et al., 2017), and further filtered or augmented by humans or existing LLMs (*e.g.,* GPT-4 (Achiam et al., 2023)).

General scientific LLMs are usually evaluated on common NLP tasks, such as named entity recognition (NER), relation extraction (RE) (Luan et al., 2018), question answering (QA) (Wang et al., 2024f), and classification (Cohan et al., 2019).

2.2 Language + Graph

Beyond plain text, scientific papers are associated with rich metadata including venues, authors, and references (Zhang et al., 2023g). Such metadata connect papers into a graph that complements text signals for characterizing paper semantics. To exploit metadata, some studies (TYPE 1.B, *e.g.,* OAG-BERT (Liu et al., 2022b)) concatenate paper text with venues/authors as input and perform MLM on both text and metadata; others (TYPE 3.A, *e.g.,* SPECTER (Cohan et al., 2020)) take citation links as supervision and train LLMs to encode linked papers closer in the embedding space. Recent approaches further modify the Transformer architecture in LLMs with Adapters (Singh et al., 2023), GNN-nested Transformers (Jin et al., 2023b), and Mixture-of-Experts Transformers (Zhang et al., 2023f) to better capture graph signals.

Graph-aware scientific LLMs are often evaluated on tasks regarding the relation between two text units (*e.g.,* paper-paper or query-paper), including link prediction, retrieval, recommendation, and author name disambiguation. SciDocs (Cohan et al., 2020) and SciRepEval (Singh et al., 2023) are widely adopted benchmark datasets.

2.3 Applications in Scientific Discovery

Performant scientific LLMs can work alongside researchers throughout the entire scientific discovery process. Leaving field-specific applications for later sections, here we underscore LLMs' general usefulness in brainstorming and evaluation: Lahav et al. (2022) integrate LLMs into a search engine for the discovery of scientific challenges and directions; Wang et al. (2023e), Yang et al. (2024d), Baek et al. (2024), Gu and Krenn (2024), and Si et al. (2024) leverage LLMs to generate novel scientific ideas, directions, and hypotheses on the basis of prior literature and existing knowledge; Zhang et al. (2023h) rely on LLMs to find expert reviewers for each submission; Liu and Shah (2023), Liang et al. (2024c), and D'Arcy et al. (2024) explore the capacity of GPT-4 to provide useful feedback on research papers to facilitate automatic review generation; Liang et al. (2024b,a) also observe the increasing use of LLMs in writing scientific papers and conference peer reviews.

3 LLMs in Mathematics (Table A2)

3.1 Language

The pre-training text corpora for mathematics LLMs can be categorized into two classes: (1) multiple-choice QA, the representative datasets of which include MathQA (Amini et al., 2019), Ape210K (Zhao et al., 2020), and Math23K (Wang et al., 2017); as well as (2) generative QA, the representative datasets of which include GSM8K (Cobbe et al., 2021), MATH (Hendrycks et al., 2021b), and MetaMathQA (Yu et al., 2024c).

Similarly to general science LLMs, the backbone model of pioneering mathematics LLMs is BERT (TYPE 1.A, *e.g.,* GenBERT (Geva et al., 2020) and MathBERT (Shen et al., 2021)), and these models are mostly trained via MLM. For GPT-based mathematics LLMs (TYPE 2.A, *e.g.,* GSM8K-GPT (Cobbe et al., 2021) and NaturalProver (Welleck et al., 2022)), next token prediction and instruction tuning are major pre-training tasks to generate mathematical proofs and reasoning processes. The most recent models (TYPE 2.A, *e.g.,* Rho-Math (Lin et al., 2024b) and MAmmoTH2 (Yue et al., 2024c)) are based on LLaMA and are trained to follow natural language instructions. However, when an enormous pre-training corpus is available (*e.g.,* mathematical web pages and code), next token prediction is still favored as the mere pre-training task (Azerbayev et al., 2024; Lin et al., 2024b) or the companion task (Shao et al., 2024; Ying et al., 2024) to build base models.

QA and math world problems (MWP) have been the most common evaluation tasks for mathematics LLMs. In addition, quantitative reasoning contains more difficult problems, as the model has to provide a complete and self-contained solution without relying on external tools (Shao et al., 2024; Lin et al., 2024b). We see a dominance of use from GSM8K and MATH for QA, and from MathQA and Math23K for MWP. For quantitative reasoning, MMLU-STEM (Hendrycks et al., 2021a) and Big-Bench Hard (Suzgun et al., 2023) are the most widely adopted.

3.2 Language + Vision

Geometry is one of the most important branches of mathematics, and it expresses the settings jointly in text and diagrams. As such, it is mandatory to involve the vision modality for geometry LLMs. The most commonly used pre-training datasets for geometry LLMs include Geometry3K (Lu et al., 2021) and GeoQA (Chen et al., 2021), both of which contain multiple-choice geometry problems.

The key to incorporating the vision modality into LLMs is to encode the images and obtain linearized visual representations. Specifically, Inter-GPS (Lu et al., 2021) (TYPE 2.D) uses RetinaNet (Lin et al., 2017) to transform images into a set of relationships and then applies BART (Lewis et al., 2020a) to produce the solution; G-LLaVA (Gao et al., 2023) (TYPE 2.D) encodes visual input via a pre-trained vision Transformer (ViT), concatenates visual embeddings with textual embeddings, and then feeds the concatenation into LLaMA-2 (Touvron et al., 2023b). These models are by default pre-trained via sequence-to-sequence tasks, where the problem is the input, and the ground-truth answer with optional rationale is the output. Auxiliary loss such as masked image modeling, image construction, or text-image matching, is optionally added for better visual modeling.

Geometry LLMs are evaluated through geometry problem solving, where the model is asked to select the correct answer given the diagram and its caption, the question, and answer options. Renowned evaluation datasets include Geometry3K (Lu et al., 2021), GEOS (Seo et al., 2015), and MathVista (Lu et al., 2024).

3.3 Table

A large proportion of math knowledge is stored in the form of tabular data. For the “Table” modality, notable resources for pre-training include WikiTableQuestions (Pasupat and Liang, 2015), WikiSQL (Zhong et al., 2017), and WDC Web Table (Lehmberg et al., 2016).

The challenge in tables is similar to that in diagrams, namely to obtain linearized table representations. In most cases, tables are squeezed into linear text sequences as part of the context and are prepended with the question text as the model input. As one of the first works in this line of research, TAPAS (Herzig et al., 2020) (TYPE 1.A) adopts the MLM objective to predict the masked token in both textual and tabular contexts. Recent developments (Li et al., 2024b; Zhang et al., 2024f) resemble the design of TableLlama (Zhang et al., 2024e) (TYPE 2.B), with LLaMA-2 as the backbone and instruction tuning as the pre-training task.

Table LLMs are validated through table QA, where the model is asked to produce the correct answer given the table structure, data values, and a question text. Most existing studies have been evaluated on the WikiTableQuestions and WikiSQL datasets. TableInstruct (Zhang et al., 2024e) is the most recently developed comprehensive benchmark integrating 14 datasets across 11 tasks.

3.4 Applications in Scientific Discovery

Mathematics LLMs have great potential to assist humans in offering potential solutions. For instance, AlphaGeometry (Trinh et al., 2024) combines an LLM with a symbolic deduction engine, where the LLM generates useful constructs and the symbolic engine applies formal logic to find solutions. AlphaGeometry solves 25 out of 30 classical geometry problems adapted from the International Mathematical Olympiad. Sinha et al. (2024) extend AlphaGeometry by adding Wu’s method (Chou, 1988), further solving 27 out of 30, surpassing human gold medalists. FunSearch (Romera-Paredes et al., 2024) integrates LLM with program search. One notable achievement of FunSearch is its ability to find a new solution to the cap set problem in combinatorial optimization. The solutions generated can be faster and more efficient than those devised by human experts. In Li et al.

(2024a), LLMs iteratively propose and critique statistical models by leveraging in-context learning and chain-of-thought reasoning (Wei et al., 2022b).

4 LLMs in Physics (Table A3)

4.1 Language

As a derivative of BERT, astroBERT (Grezes et al., 2024) (TYPE 1.A) is further pre-trained using astronomy-related papers via MLM and next sentence prediction. It is evaluated on the NER task. Likewise, AstroLLaMA (Nguyen et al., 2023b) (TYPE 2.A) fine-tunes LLaMA-2 using over 300,000 astronomy abstracts from arXiv. It is evaluated on paper generation and recommendation tasks. AstroLLaMA-chat (Perkowski et al., 2024) (TYPE 2.A) is the chat version of AstroLLaMA. It is continually trained on a GPT-4 generated domain-specific dialogue dataset. PhysBERT (Hellert et al., 2024) (TYPE 1.A) is the first physics-specific model for sentence embedding trained on a curated corpus of physics literature based on 1.2 million physics papers on arXiv. It is evaluated on physics-tailored tasks, such as information retrieval, classification, and semantic similarity estimation.

4.2 Applications in Scientific Discovery

Transformer-based physics LLMs can potentially assist humans in solving differential equations and designing experiments. For instance, Cai et al. (2024) apply Transformer to predict the integer coefficients in the scattering amplitudes of Planar $\mathcal{N} = 4$ Super Yang-Mills theory; RydbergGPT (Fitzek et al., 2024) uses Transformer to learn the distribution of qubit measurement outcomes that describe an array of interacting Rydberg atoms; Arlt et al. (2024) present an initial trial that applies a code-generating LLM to synthesize experimental blueprints for a whole class of quantum systems in the form of Python code.

5 LLMs in Chemistry and Materials Science (Table A4)

5.1 Language

LLM pre-training corpora in chemistry and materials science typically come from research papers and databases (*e.g.,* Materials Project (Jain et al., 2013)). Besides, recent works adopt domain-specific instruction tuning datasets (e.g., Mol-Instructions (Fang et al., 2024a) and SMolInstruct (Yu et al., 2024a)) derived from PubChem (Kim et al., 2019), MoleculeNet (Wu et al., 2018), *etc.*

Early studies on chemistry LLMs mostly adopt a moderate-sized encoder-only architecture pre-trained with MLM (TYPE 1.A, *e.g.,* ChemBERT (Guo et al., 2022), MatSciBERT (Gupta et al., 2022), and BatteryBERT (Huang and Cole, 2022)). These models are usually evaluated on downstream tasks including reaction role labeling (Guo et al., 2022) and abstract classification (Gupta et al., 2022). Recently, researchers have focused more on large-scale decoder-only LLMs trained with next token prediction and instruction tuning (TYPE 2.A). Examples include ChemDFM (Zhao et al., 2024), ChemLLM (Zhang et al., 2024b), and LlaSMol (Yu et al., 2024a). Given the desired generalization capability of such models, they are evaluated on a diverse set of tasks such as name conversion (Kim et al., 2019), reaction prediction (Jin et al., 2017), retrosynthesis (Schneider et al., 2016), text-based molecule design (Edwards et al., 2022), and crystal generation (Antunes et al., 2023; Flam-Shepherd and Aspuru-Guzik, 2023; Gruver et al., 2024).

5.2 Language + Graph

Graphs are appropriate data structures for characterizing molecules (Jin et al., 2023a). Popular datasets containing molecular graphs include ChEBI-20 (Edwards et al., 2021, 2022), ZINC (Sterling and Irwin, 2015), and PCDes (Zeng et al., 2022).

In some scenarios, molecular graphs appear simultaneously with text information, thus existing works have explored how to encode both effectively. The first type of such models adopts a GNN as the graph encoder and an LLM as the text encoder. The two modalities are connected through contrastive learning (Liu et al., 2023d) (TYPE 3.C). For example, Text2Mol (Edwards et al., 2021) uses GCN (Kipf and Welling, 2017) and SciBERT to encode a molecule and its corresponding natural language description, respectively, for text-to-molecule retrieval. The second type of such models utilizes an LLM to encode text and graphs simultaneously (Zeng et al., 2022). Graphs can be either linearized to SMILES strings (Edwards et al., 2022) (TYPE 2.C) or projected onto virtual tokens with graph encoders (Zhao et al., 2023a; Liu et al., 2023e) (TYPE 2.D). For instance, 3D-MoLM (Li et al., 2024c) uses a 3-dimensional molecular encoder to represent molecules as tokens and feeds them together with instructions into LLaMA-2 for molecule-to-text retrieval and molecule captioning.

5.3 Language + Vision

Complementing text and graph modalities, molecular images form the vision modality in chemistry. Existing works adopt a similar philosophy to BLIP-2 (Li et al., 2023b), which represents each image as tokens and feeds them into an LLM (TYPE 2.D). For example, GIT-Mol (Liu et al., 2024a) projects all modalities, including graphs and images, into the latent text space and conducts encoding and decoding using T5 (Raffel et al., 2020).

5.4 Molecule

Different from subsection 5.2, this subsection introduces models dealing with molecules without associated text information. That being said, comparable approaches inspired by LLMs are utilized to develop molecular language models (Flam-Shepherd et al., 2022). To be specific, most studies adopt SMILES or SELFIES (Krenn et al., 2020) strings as the sequential representation of molecules. Similar to the trend in the "Language" modality, pioneering molecular LLMs focus on representation learning with bidirectional Transformer encoders (TYPE 1.C, *e.g.,* SMILES-BERT (Wang et al., 2019) and MoLFormer (Ross et al., 2022)). For instance, ChemBERTa (Chithrananda et al., 2020) adopts the architecture and pre-training strategy similar to those of RoBERTa (Liu et al., 2019). These models exhibit extraordinary abilities in molecular understanding tasks such as molecular property prediction (*e.g.,* toxicity classification (Wu et al., 2018) and atomization energy regression (Ramakrishnan et al., 2014)) as well as virtual screening (Riniker and Landrum, 2013). Later works explore the idea of representing molecules in an autoregressive fashion (TYPE 2.C, *e.g.,* BARTSmiles (Chilingaryan et al., 2024) and ChemGPT (Frey et al., 2023)). For instance, T5Chem (Lu and Zhang, 2022) adopts the T5 backbone and a sequence-to-sequence pre-training objective. These models are evaluated in generative tasks that include molecule generation (Gaulton et al., 2017), reaction prediction, and retrosynthesis. Besides linearizing molecules, there are studies modifying the Transformer architecture to admit molecular graphs, such as MAT (Maziarka et al., 2020) and R-MAT (Maziarka et al., 2024).

5.5 Applications in Scientific Discovery

Previous studies have shown that LLMs facilitate autonomous chemical research. For example, Bran et al. (2024) present a chemistry LLM agent, ChemCrow, that can integrate expert-designed tools for organic synthesis, drug discovery, and materials design; Zheng et al. (2023a) demonstrate that LLMs can perform knowledge synthesis from the scientific literature, knowledge inference from data, and interpretable explanation generation in chemistry; Boiko et al. (2023) develop an LLM-empowered intelligence system, Coscientist, that can design, plan, and perform chemical research. Moreover, LLMs accomplish complex tasks in chemistry, such as drug and catalyst design and molecular discovery, purely from instructions (White, 2023). For instance, Ramos et al. (2023) study catalyst and molecule design with in-context learning, removing the requirement for traditional training or simulation processes; ChatDrug (Liu et al., 2024b) explores drug editing using LLMs with a prompt module, a domain feedback module, and a conversation module; Jablonka et al. (2024) find that fine-tuned LLMs perform comparably to, or even better than, conventional techniques for many chemistry applications, spanning from the properties of molecules and materials to the yield of chemical reactions; DrugAssist (Ye et al., 2023a) serves as an LLM-based interactive model for molecule optimization through human-machine dialogue; Sprueill et al. (2023, 2024) use LLMs as agents to search for effective catalysts through Monte Carlo Tree Search and the feedback from an atomistic neural network model; Wang et al. (2024b) re-engineer crossover and mutation operations for molecular discovery using LLMs trained on extensive chemical datasets. Meanwhile, benchmarking studies by Mirza et al. (2024) demonstrate that although LLMs achieve superhuman proficiency in many chemical tasks, further research is critical to enhancing their safety and utility in chemical sciences.

6 LLMs in Biology and Medicine (Table A5)

6.1 Language

Besides research articles (*e.g.,* titles/abstracts from PubMed (Lu, 2011) and full text from PMC (Beck and Sequeira, 2003)), pre-training corpora for biomedical LLMs include electronic health records (*e.g.,* MIMIC-III (Johnson et al., 2016), MIMIC-IV (Johnson et al., 2023)), knowledge bases (e.g., UMLS (Bodenreider, 2004)), and health-related social media posts (*e.g.,* COVID-19 tweets (Müller et al., 2023)). Recent studies further collect supervised fine-tuning and preference optimization datasets from medical exam questions, knowledge graphs, and doctor-patient dialogues. Examples include ChiMed (Ye et al., 2023b), MedInstruct-52k (Zhang et al., 2023d), and BiMed1.3M (Acikgoz et al., 2024), many of which have non-English components (*e.g.,* Chinese and Arabic).

The watershed moment in the evolution biomedical LLMs is still the emergence of billion-parameter architectures and instruction tuning. Before that, a wide variety of moderate-sized backbones are explored, including both encoder-based (Type 1.a, *e.g.,* BioBERT (Lee et al., 2020), BioELECTRA (Ozyurt, 2020), BioRoBERTa (Lewis et al., 2020b), BioALBERT (Naseem et al., 2022), and Clinical-Longformer (Li et al., 2022a)) and (encoder-)decoder-based ones (Type 2.a, *e.g.,* SciFive (Phan et al., 2021), BioBART (Yuan et al., 2022a), and BioGPT (Luo et al., 2022)). Evaluation tasks for these models range from biomedical NER, RE, sentence similarity estimation, document classification, and QA (*i.e.,* the BLURB benchmark (Gu et al., 2021)) to natural language inference (NLI) (Romanov and Shivade, 2018) and entity linking (Doğan et al., 2014). After the watershed, the trend becomes instruction-tuning billion-parameter LLMs (Type 2.a, *e.g.,* Med-PaLM (Singhal et al., 2023a), MedAlpaca (Han et al., 2023), and BioMistral (Labrak et al., 2024)). Accordingly, evaluation tasks now include single-round QA (Jin et al., 2021; Pal et al., 2022) and multi-round dialogue (Wang et al., 2024g). Meanwhile, there are studies proposing a Bi-Encoder architecture (Type 3.a, *e.g.,* Jin et al. (2023c) and Xu et al. (2024)) that specifically targets biomedical retrieval tasks, the benchmarks of which are NFCorpus (Boteva et al., 2016), TREC-COVID (Voorhees et al., 2021), *etc.*

6.2 Language + Graph

Biomedical ontologies capture rich types of relations between entities. Analogously, citation links characterize connections between biomedical papers. Intuitively, jointly leveraging text and such graph information paves the way for multi-hop reasoning in QA. For instance, Yasunaga et al. (2022a) propose to use an LLM and a GNN to encode text and ontology signals, respectively, and deeply fuse them (Type 3.c); Yasunaga et al. (2022b) concatenate text segments from two linked papers together and feed the sequence into an LLM for pre-training, which is essentially appending a metadata neighbor (*i.e.,* reference) as context for MLM (Type 1.b). Both approaches demonstrate significant improvement in QA tasks that require complex reasoning.

6.3 Language + Vision

Biomedical text-image pairs typically come from two sources: (1) medical reports, such as chest X-rays (*e.g.,* MIMIC-CXR (Johnson et al., 2019)) and pathology reports (Huang et al., 2023); as well as (2) figure-caption pairs extracted from biomedical papers (*e.g.,* ROCO (Pelka et al., 2018) and MedICaT (Subramanian et al., 2020)).

Most biomedical vision-language models exploit the CLIP architecture (Radford et al., 2021), where a text encoder and an image encoder are jointly trained to map the paired text and image closer via contrastive learning (Type 3.d). The choice of the text encoder evolves from BERT (Zhang et al., 2022) and GPT-2 (Huang et al., 2023) to LLaMA (Wu et al., 2023) and LLaMA-2 (Liu et al., 2023b), while the image encoder evolves from ResNet (Huang et al., 2021) to ViT (Zhang et al., 2023c) and Swin Transformer (Thawkar et al., 2024). MLM, masked image modeling, and text-text/image-image contrastive learning (*i.e.,* by creating augmented views within the language/vision modality) are sometimes adopted as auxiliary pre-training tasks. Besides CLIP, other general-domain vision-language architectures, such as LLaVA (Li et al., 2023a), PaLM-E (Tu et al., 2024), and Gemini (Saab et al., 2024), have been explored. For instance, LLaVA-Med (Type 2.d) encodes images onto several visual tokens and prepends them to text tokens as the LLM input. Evaluation tasks of these models encompass image classification, segmentation, object detection, vision QA, text-to-image/image-to-text retrieval, and report generation, the benchmarks of which include CheXpert (Irvin et al., 2019), PadChest (Bustos et al., 2020), SLAKE (Liu et al., 2021a), *etc.*

6.4 Protein, DNA, RNA, and Multiomics

The FASTA format (Lipman and Pearson, 1985) naturally represents proteins as amino acid sequences and DNAs/RNAs as nucleotide sequences, enabling models to treat them as "languages". Representative resources of such sequences include UniRef (Suzek et al., 2015) and Swiss-Prot (Bairoch and Apweiler, 2000) for proteins, GRCh38 (Harrow et al., 2012) and the 1000 Genomes Project (Consortium, 2015) for DNAs, as well as RNAcentral (Consortium, 2019) for RNAs.

Encoder-only protein, DNA, and RNA LLMs (Type 1.d), such as ESM-2 (Lin et al., 2023b), DNABERT (Ji et al., 2021), and RNABERT (Akiyama and Sakakibara, 2022), adopt BERT-like architectures and MLM as the pre-training task (*i.e.*, predicting masked amino acids, nucleotides, k-mers, or codons); decoder-only models, such as ProGen (Madani et al., 2023) and DNAGPT (Zhang et al., 2023a), exploit GPT-like architectures and next token prediction as the pre-training task. There are also studies jointly considering text and protein modalities. For instance, ProtST (Xu et al., 2023b) matches protein sequences with their text descriptions (*i.e.,* names and functions) via contrastive learning (Type 3.b); BioMedGPT

(Luo et al., 2023c) first projects proteins onto tokens and then inputs these tokens together with text into LLaMA-2 for instruction tuning, bearing similarity with TYPE 2.D.

Existing multiomics LLMs mainly focus on single-cell transcriptomics (*e.g.,* scRNA-seq) data, such as the expression levels of genes within a single cell (Franzén et al., 2019). Besides BERT-based (*e.g.,* Geneformer (Theodoris et al., 2023)) and GPT-based (*e.g.,* scGPT (Cui et al., 2024)) architectures, Performer (Yang et al., 2022a; Hao et al., 2024) is widely used due to its linear attention complexity in handling long scRNA-seq data.

6.5 Applications in Scientific Discovery

Similarly to chemistry, LLMs can automate experiments in biological and medical research. For example, CRISPR-GPT (Huang et al., 2024a) augments an LLM agent with domain knowledge to enhance the design process of CRISPR-based gene-editing experiments; TrialMind (Wang et al., 2024h) utilizes LLMs to extract results and synthesize clinical evidence from the literature for medical discovery. Moreover, LLMs can encode biological sequences to capture structural properties and guide protein design. For instance, ESM-1b (Rives et al., 2021) and ESM-2 (Lin et al., 2023b) enable accurate structure prediction of proteins without expensive and time-consuming experiments; Ferruz and Höcker (2022) fine-tune LLMs on protein families, which can generate highly divergent but still potentially functional novel sequences; He et al. (2024a) leverage an LLM for the de novo generation of SARS-CoV-2 antibodies with desired antigen-binding specificity; Hie et al. (2021) develop LLMs to evaluate the evolutionary fitness of viral variants using sequence data alone.

7 LLMs in Geography, Geology, and Environmental Science (Table A6)

7.1 Language

Geoscience research papers, climate-related news articles, Wikipedia pages, corporate sustainability reports, knowledge bases (*e.g.,* GAKG (Deng et al., 2021)), and point-of-interest (POI) data (*e.g.,* OpenStreetMap (Haklay and Weber, 2008)) constitute the pre-training corpora for geoscience LLMs.

Preliminary research on geoscience LLMs focuses on pre-training bidirectional LLMs with the Transformer encoder backbone (TYPE 1.A, *e.g.,* ClimateBERT (Webersinke et al., 2021), SpaBERT (Li et al., 2022b), and MGeo (Ding et al., 2023)). For instance, SpaBERT and MGeo perform MLM on a sequence of geolocations for geographic entity linking and query-POI matching, respectively. More recently, related studies concentrate on scaling up decoding-style autoregressive LLMs in geoscience (TYPE 2.A, *e.g.,* K2 (Deng et al., 2024), OceanGPT (Bi et al., 2023b), and GeoGalactica (Lin et al., 2024c)). For instance, K2 and OceanGPT adapt LLaMA to geoscience and ocean science, respectively, via supervised fine-tuning with domain-specific instructions curated by human experts and/or augmented by general-domain LLMs. Evaluations of such models are conducted on geoscience benchmarks, such as GeoBench (Deng et al., 2024) and OceanBench (Bi et al., 2023b), which encompass a broad range of tasks including QA, classification, knowledge probing, reasoning, summarization, and generation.

7.2 Language + Graph

Some geoscience applications involve graph signals, such as heterogeneous POI networks and knowledge graphs. To handle such signals and text jointly, ERNIE-GeoL (Huang et al., 2022) introduces a Transformer-based aggregation layer to deeply fuse text and POI information within a BERT-based architecture; PK-Chat (Deng et al., 2023) combines an LLM with a pointer generation network on a knowledge graph to build a knowledge-driven dialogue system.

7.3 Language + Vision

Aerial views, together with location descriptions, profile urban regions. To address language and vision modalities jointly, UrbanCLIP (Yan et al., 2024) considers the CLIP architecture (TYPE 3.D), which is also widely adopted by biomedical vision-language models as mentioned in subsection 6.3, to perform text-image contrastive learning for urban indicator prediction.

7.4 Climate Time Series

The intuitions and methodologies used in LLMs also facilitate the construction of climate foundation models. Based on the ERA5 (Hersbach et al., 2020) and CMIP6 (Eyring et al., 2016) datasets of climate time series, previous studies exploit the ViT and Swin Transformer architectures to pre-train foundation models for weather forecasting. Representative models include FourCastNet (Pathak et al., 2022), Pangu-Weather (Bi et al., 2023a), *etc.*

7.5 Applications in Scientific Discovery

In geography, Wang et al. (2023b) and Zhou et al. (2024b) highlight the potential of LLMs in urban planning from sustainability, living, economic, disaster, and environmental perspectives. In geology, besides climate and weather forecasting, foundation models have been applied to simultaneous earthquake detection and phase picking (Mousavi et al., 2020). In environmental science, ChatClimate (Vaghefi et al., 2023) enhances GPT-4 by providing access to external, scientifically accurate knowledge on climate change to build a climate science conversational AI.

8 Challenges and Future Directions

In this survey, we compile literature that elucidates the data, architectures, and tasks used for scientific LLM pre-training, as well as how scientific LLMs have been applied to downstream applications in scientific discovery. In particular, we underscore analogous architectures, tasks, and trends observed during the evolution of scientific LLMs across different fields and modalities. Beyond reviewing prior research, we present several challenges to inspire further exploration of this topic.

Diving into Fine-Grained Themes. Most existing scientific LLMs target a coarse-grained field (*e.g.,* chemistry), while some tasks rely on highly specialized knowledge of a fine-grained theme (*e.g.,* Suzuki coupling). When LLMs are pre-trained on more general corpora, frequently appeared signals may dominate the model parameter space, and domain-specific tail knowledge may be wiped out. We believe that automatically curating in-depth, theme-focused knowledge graphs (Hope et al., 2021) to guide the generation process will be a promising direction to tackle this issue.

Generalizing to Out-of-Distribution Scientific Data. In the scientific domain, it is common that the testing distribution shifts from the training distribution (Zhang et al., 2023e): novel scientific concepts keep emerging in newly published papers; unseen molecules with different scaffolds and unseen proteins with different numbers of peptide chains may appear during testing. Handling such out-of-distribution data remains a challenge for pre-trained scientific LLMs. To our knowledge, invariant learning (Arjovsky et al., 2019) can serve as the theoretical foundation for out-of-distribution analyses, and how to integrate it into LLM pre-training is worth exploring.

Facilitating Trustworthy Predictions. LLMs can generate plausible-sounding but factually incorrect output, commonly known as hallucination (Ji et al., 2023), which is particularly dangerous in high-stakes scientific domains such as chemistry and biomedicine. To mitigate this issue, retrieval-augmented generation (RAG) provides LLMs with relevant, up-to-date, and trustworthy information. However, previous RAG studies in the scientific domain mainly focus on retrieving text (Xiong et al., 2024) and knowledge (Jin et al., 2024), while scientific data are heterogeneous and multi-modal. We envision that cross-modal RAG (*e.g.,* guiding text generation with relevant chemicals and proteins) will present additional opportunities to further enhance the trustworthiness of scientific LLMs.

Limitations

This survey primarily covers LLMs in mathematics and natural sciences. We are aware that LLMs can also significantly impact social sciences by achieving remarkable performance in representative tasks (Ziems et al., 2024) and serving as agents for social simulation experiments (Horton, 2023), but we leave the survey of these efforts as future work due to space limitations. In addition, this paper focuses on LLMs pre-trained on scientific data or augmented with domain-specific knowledge to benefit scientific discovery. There are studies (Guo et al., 2023; Wang et al., 2024f; Yue et al., 2024a; Liang et al., 2024d) proposing new benchmark datasets of scientific problems but evaluating the performance of general-purpose LLMs only, and we do not include these works in our survey. Furthermore, some LLMs may belong to more than one field or modality category given our classification criteria in the paper. For instance, BioMedGPT (Luo et al., 2023c) is pre-trained on biology and chemistry data jointly; GIT-Mol (Liu et al., 2024a) considers the language, graph, and vision modalities simultaneously. For the sake of brevity, we introduce each of them in only one subsection.

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A Summary Tables of Scientific LLMs

Table A1-Table A6 summarize the modality, number of parameters, model architecture, pre-training data, pre-training task(s), and evaluation task(s) of scientific LLMs in each field. Within each field, we categorize models according to their modality; within each modality, we sort models chronologically. To be specific, if a paper has a preprint (*e.g.,* arXiv or bioRxiv) version, its publication date is according to the preprint service. Otherwise, its publication date is according to the conference proceeding or journal.

Table A1: Summary of LLMs in general science. "L": Language; "L+G": Language + Graph; "∼": generally adopting the architecture but with modifications; "MLM": masked language modeling; "NSP": next sentence prediction; "NER": named entity recognition; "RE": relation extraction; "QA": question answering.

Model	**Modality**	**Size**	**Architecture**	**Pre-training Data**	**Pre-training Task(s)**	**Evaluation Task(s)**
SciBERT (Beltagy et al., 2019)	L	110M	BERT	Semantic Scholar	MLM, NSP	NER, RE, classification, parsing
SciGPT2 (Luu et al., 2021)	L	117M	GPT-2	S2ORC	next token prediction	paper relationship explanation
CATTS (Cachola et al., 2020)	L	406M	BART	SciTLDR	sequence to sequence	summarization
SciNewsBERT (Smeros et al., 2021)	L	110M	BERT	news headlines	MLM, NSP	scientific claim extraction
ScholarBERT (Hong et al., 2023)	L	340M, 770M	BERT	Public.Resource.Org, Wikipedia, BookCorpus	MLM	NER, RE, classification
AcademicRoBERTa (Yamauchi et al., 2022)	L	125M	RoBERTa	CiNii	MLM	classification, author identification
Galactica (Taylor et al., 2022)	L	125M, 1.3B, 6.7B, 30B, 120B	Galactica	papers, code, reference materials, knowledge bases, web crawl data, instructions	next token prediction, instruction tuning	QA, link prediction, knowledge probing, quantitative reasoning, chemical name conversion, molecule classification, protein function prediction
DARWIN (Xie et al., 2023)	L	7B	LLaMA	papers, QA pairs, instructions	instruction tuning	QA, classification, regression
FORGE (Yin et al., 2023)	L	1.4B, 13B, 22B	GPT-NeoX	CORE, AMiner, MAG, SCOPUS, arXiv	next token prediction	QA, classification, regression
SciGLM (Zhang et al., 2024a)	L	6B, 32B	ChatGLM	SciInstruct	instruction tuning	QA, quantitative reasoning
SPECTER (Cohan et al., 2020)	L+G	110M	BERT	Semantic Scholar	link prediction	classification, link prediction, recommendation
OAG-BERT (Liu et al., 2022b)	L+G	110M	∼BERT	AMiner, PubMed, OAG	MLM	classification, link prediction, recommendation, retrieval, author name disambiguation
ASPIRE (Mysore et al., 2022)	L+G	110M	BERT	S2ORC	link prediction	paper similarity estimation
SciNCL (Ostendorff et al., 2022)	L+G	110M	BERT	Semantic Scholar	link prediction	classification, link prediction, recommendation
SPECTER 2.0 (Singh et al., 2023)	L+G	113M	Adapters	SciRepEval	classification, regression, link prediction, retrieval	classification, regression, link prediction, retrieval, author name disambiguation, paper-reviewer matching
SciPatton (Jin et al., 2023b)	L+G	–	GraphFormers	MAG	MLM, link prediction	classification, link prediction
SciMult (Zhang et al., 2023f)	L+G	138M	MoE	MAG, Semantic Scholar, SciRepEval	classification, link prediction, retrieval	classification, link prediction, recommendation, retrieval, patient-article/patient matching

Table A2: Summary of LLMs in mathematics. "L+V": Language + Vision; "MWP": math word problems. Other notations have the same meaning as in previous tables.

Model	**Modality**	**Size**	**Architecture**	**Pre-training Data**	**Pre-training Task(s)**	**Evaluation Task(s)**
GenBERT (Geva et al., 2020)	L	110M	BERT	Wikipedia	MLM, sequence to sequence	QA, MWP
MathBERT (Shen et al., 2021)	L	110M	BERT	arXiv, math curricula, syllabi, textbooks	MLM	classification, auto-grading
MWP-BERT (Liang et al., 2022)	L	110M	BERT	Ape210K	MLM, regression, classification	QA, MWP
BERT-TD (Li et al., 2022c)	L	110M	BERT	Math23K, MathQA	sequence to sequence, contrastive learning	QA, MWP
GSM8K-GPT (Cobbe et al., 2021)	L	6B, 175B	GPT-3	GSM8K	supervised fine-tuning	QA, MWP
DeductReasoner (Jie et al., 2022)	L	125M	RoBERTa	MAWPS, Math23K, MathQA, SVAMP	sequence to sequence	QA, MWP
NaturalProver (Welleck et al., 2022)	L	175B	GPT-3	NaturalProofs	supervised fine-tuning	mathematical proof generation
Minerva (Lewkowycz et al., 2022)	L	8B, 62B, 540B	PaLM	arXiv, math web pages	next token prediction	QA, MWP, quantitative reasoning
Bhāskara (Mishra et al., 2022)	L	2.7B	GPT-Neo	Līla	instruction tuning	QA, MWP, knowledge probing
WizardMath (Luo et al., 2023a)	L	7B, 13B, 70B	LLaMA-2	GSM8K, MATH	instruction tuning	QA, MWP
MAmmoTH (Yue et al., 2024b)	L	7B, 13B, 34B, 70B 7B	LLaMA-2 Mistral	MathInstruct	instruction tuning	QA, MWP
MetaMath (Yu et al., 2024c)	L	7B, 13B, 70B 7B	LLaMA-2 Mistral	MetaMathQA	instruction tuning	QA, MWP
ToRA (Gou et al., 2024)	L	7B, 13B, 34B, 70B	LLaMA-2	ToRA-Corpus	instruction tuning	QA, MWP
MathCoder (Wang et al., 2024c)	L	7B, 13B, 34B, 70B	LLaMA-2	MathCodeInstruct	instruction tuning	QA, MWP

(Mathematics, Table Continued)

Model	Modality	Size	Architecture	Pre-training Data	Pre-training Task(s)	Evaluation Task(s)
Llemma (Azerbayev et al., 2024)	L	7B, 34B	LLaMA-2	Proof-Pile-2	next token prediction	QA, MWP, quantitative reasoning
OVM (Yu et al., 2024b)	L	7B 7B	LLaMA-2 Mistral	GSM8K	supervised fine-tuning	QA, MWP, quantitative reasoning
DeepSeekMath (Shao et al., 2024)	L	7B	DeepSeek	math web pages, instructions	next token prediction, instruction tuning	QA, MWP, quantitative reasoning, formal translation
InternLM-Math (Ying et al., 2024)	L	7B, 20B	InternLM2	Knowledge Pile, Proof-Pile-2, instructions	next token prediction, instruction tuning	QA, MWP, quantitative reasoning, formal translation
OpenMath (Toshniwal et al., 2024)	L	7B, 13B, 34B, 70B 7B	LLaMA-2 Mistral	OpenMathInstruct-1	instruction tuning	QA, MWP
Rho-Math (Lin et al., 2024b)	L	1B 7B	∼LLaMA-2 Mistral	OpenWebMath, SlimPajama, StarCoderData	next token prediction	QA, MWP, quantitative reasoning
MAmmoTH2 (Yue et al., 2024c)	L	8B 7B 8×7B	LLaMA-3 Mistral Mixtral	WebInstruct	instruction tuning	QA, MWP, quantitative reasoning
TheoremLlama (Wang et al., 2024e)	L	8B	LLaMA-3	Open Bootstrapped Theorems	instruction tuning	mathematical proof generation
Inter-GPS (Lu et al., 2021)	L+V	–	∼BART + RetinaNet	Geometry3K, GEOS	sequence to sequence	geometry problem solving
Geoformer (Chen et al., 2022a)	L+V	–	VL-T5 + ResNet	UniGeo	sequence to sequence	geometry problem solving
SCA-GPS (Ning et al., 2023)	L+V	–	RoBERTa + ViT	GeoQA, Geometry3K	masked image modeling, sequence to sequence	geometry problem solving
UniMath-Flan-T5 (Liang et al., 2023)	L+V	–	Flan-T5 + VQ-VAE	SVAMP, GeoQA, TabMWP	image reconstruction, sequence to sequence	MWP, geometry problem solving
G-LLaVA (Gao et al., 2023)	L+V	7B, 13B	LLaVA	GeoQA+, Geometry3K	text-image matching, instruction tuning	geometry problem solving
TAPAS (Herzig et al., 2020)	Table	110M, 340M	BERT	Wikipedia	MLM	table QA
TaBERT (Yin et al., 2020)	Table	110M, 340M	BERT	Wikipedia, WDC Web Table	MLM, cell value recovery	table QA
GraPPa (Yu et al., 2021)	Table	355M	RoBERTa	Wikipedia	MLM, SQL semantic prediction	table QA
TUTA (Wang et al., 2021)	Table	110M	BERT	Wikipedia, WDC Web Table, spreadsheets	MLM, cell-level cloze, table context retrieval	cell type classification, table type classification
RCI (Glass et al., 2021)	Table	12M	ALBERT	WikiSQL, TabMCQ, WikiTableQuestions	classification	table QA
TABBIE (Iida et al., 2021)	Table	110M	ELECTRA	Wikipedia, VizNet	MLM, replaced token detection	column/row population, column type classification
TAPEX (Liu et al., 2022a)	Table	140M, 406M	BART	WikiTableQuestions	sequence to sequence	table QA
FORTAP (Cheng et al., 2022)	Table	110M	BERT	spreadsheets	MLM, numerical reference prediction, numerical calculation prediction	table QA, formula prediction, cell type classification
OmniTab (Jiang et al., 2022)	Table	406M	BART	Wikipedia	sequence to sequence	table QA
ReasTAP (Zhao et al., 2022)	Table	406M	BART	Wikipedia	sequence to sequence	table QA, table fact verification, table-to-text generation
Table-GPT (Li et al., 2024b)	Table	175B –	GPT-3.5 ChatGPT	instructions	instruction tuning	table QA, column-finding, missing-value identification, column type classification, data transformation, table matching, data cleaning
TableLlama (Zhang et al., 2024e)	Table	7B	LLaMA-2	TableInstruct	instruction tuning	table QA, RE, entity linking, column type classification, column/row population, table fact verification, cell description
TableLLM (Zhang et al., 2024f)	Table	7B, 13B	LLaMA-2	WikiTQ, FeTaQA, TAT-QA, WikiSQL, Spider	instruction tuning	table QA, table updating, table merging, table charting

Table A3: Summary of LLMs in physics. Notations have the same meaning as in previous tables.

Model	Modality	Size	Architecture	Pre-training Data	Pre-training Task(s)	Evaluation Task(s)
astroBERT (Grezes et al., 2024)	L	110M	BERT	NASA Astrophysics Data System	MLM, NSP	NER
AstroLLaMA (Nguyen et al., 2023b)	L	7B	LLaMA-2	arXiv	next token prediction	paper generation, paper similarity estimation
AstroLLaMA-Chat (Perkowski et al., 2024)	L	7B	LLaMA-2	QA pairs, LIMA, OpenOrca, UltraChat	instruction tuning	QA
PhysBERT (Hellert et al., 2024)	L	110M	BERT	arXiv	MLM, contrastive learning	classification, retrieval, clustering

Table A4: Summary of LLMs in chemistry and materials science. “L+G+V”: Language + Graph + Vision; “KG”: knowledge graph; “SMILES”: simplified molecular-input line-entry system. Other notations have the same meaning as in previous tables.

Model	Modality	Size	Architecture	Pre-training Data	Pre-training Task(s)	Evaluation Task(s)
ChemBERT (Guo et al., 2022)	L	110M	BERT	chemistry journals	MLM	NER
MatSciBERT (Gupta et al., 2022)	L	110M	BERT	ScienceDirect	MLM	NER, RE, classification
MatBERT (Trewartha et al., 2022)	L	110M	BERT	materials science journals	MLM	NER
BatteryBERT (Huang and Cole, 2022)	L	110M	BERT	Elsevier, Springer, RSC	MLM	QA, classification
MaterialsBERT (Shetty et al., 2023)	L	110M	BERT	materials science journals	MLM, NSP	NER
Recycle-BERT (Kumar et al., 2023)	L	110M	BERT	plastic recycling articles	classification	QA, classification
CatBERTa (Ock et al., 2023)	L	125M	RoBERTa	OC20	regression	regression
LLM-Prop (Rubungo et al., 2023)	L	37M	T5 (encoder)	Materials Project	classification, regression	classification, regression

(Chemistry and Materials Science, Table Continued)

Model	Modality	Size	Architecture	Pre-training Data	Pre-training Task(s)	Evaluation Task(s)
ChemDFM (Zhao et al., 2024)	L	13B	LLaMA	chemistry papers, textbooks, instructions	next token prediction, instruction tuning	QA, classification, name conversion, molecule captioning, text-based molecule design, reaction prediction, retrosynthesis
CrystalLLM (Gruver et al., 2024)	L	7B, 13B, 70B	LLaMA-2	Materials Project	instruction tuning	crystal generation
ChemLLM (Zhang et al., 2024b)	L	7B	InternLM2	QA pairs, ChemData	instruction tuning	QA, classification, name conversion, molecule captioning, text-based molecule design, reaction prediction, retrosynthesis
LlaSMol (Yu et al., 2024a)	L	6.7B 7B 7B	Galactica LLaMA-2 Mistral	SMolInstruct	instruction tuning	QA, classification, regression, name conversion, molecule captioning, text-based molecule design, reaction prediction, retrosynthesis
Text2Mol (Edwards et al., 2021)	L+G	–	BERT + GCN	PubChem, ChEBI-20	text-graph matching	text-to-molecule retrieval
KV-PLM (Zeng et al., 2022)	L+G	110M	BERT	S2ORC, PubChem	text-graph matching	NER, RE, classification, text-to-molecule retrieval, molecule-to-text retrieval
MolT5 (Edwards et al., 2022)	L+G	60M, 220M, 770M	T5	C4, ZINC, ChEBI-20	sequence to sequence	molecule captioning, text-based molecule design
MoMu (Su et al., 2022)	L+G	–	BERT + GIN	S2ORC, PubChem	text-graph matching	classification, text-to-molecule retrieval, molecule-to-text retrieval, molecule captioning, text-based molecule design
MoleculeSTM (Liu et al., 2023d)	L+G	–	BERT + GIN	PubChem	text-graph matching	classification, text-to-molecule retrieval, molecule-to-text retrieval, text-based molecule design
Text+Chem T5 (Christofidellis et al., 2023)	L+G	60M, 220M	T5	Pistachio, ChEBI-20, experimental procedures	sequence to sequence	molecule captioning, text-based molecule design, reaction prediction, retrosynthesis, paragraph-to-action generation
GIMLET (Zhao et al., 2023a)	L+G	60M	~T5	ChEMBL	instruction tuning	classification, regression
MolFM (Luo et al., 2023b)	L+G	–	~BERT + GIN	S2ORC, PubChem	MLM, KG embedding, text-graph matching	classification, text-to-molecule retrieval, molecule-to-text retrieval, molecule captioning, text-based molecule design
MolCA (Liu et al., 2023e)	L+G	–	Galactica + GIN	PubChem	text-graph matching, graph-to-text generation	classification, name conversion, molecule-to-text retrieval, molecule captioning, functional group counting
InstructMol (Cao et al., 2023)	L+G	–	LLaMA + GIN	PubChem, MoleculeNet, ChEBI-20, USPTO	text-graph matching, instruction tuning	classification, regression, molecule captioning, reaction prediction, retrosynthesis, reagent selection
3D-MoLM (Li et al., 2024c)	L+G	–	LLaMA-2 + Uni-Mol	PubChem, 3D-MoIT	text-graph matching, graph-to-text generation, instruction tuning	QA, regression, molecule-to-text retrieval, molecule captioning
GIT-Mol (Liu et al., 2024a)	L+G+V	–	BERT + GIN + Swin	PubChem, ChEBI-20	text-graph/image/text matching, supervised fine-tuning	classification, molecule captioning, text-based molecule design, molecule image recognition
SMILES-BERT (Wang et al., 2019)	Molecule	–	~BERT	ZINC	MLM	classification
MAT (Maziarka et al., 2020)	Molecule	–	~BERT	ZINC	masked node prediction	classification, regression
ChemBERTa (Chithrananda et al., 2020)	Molecule	125M	RoBERTa	PubChem	MLM	classification
MolBERT (Fabian et al., 2020)	Molecule	110M	BERT	ChEMBL	MLM, regression, SMILES equivalence	classification, regression, virtual screening
rxnfp (Schwaller et al., 2021b)	Molecule	110M	BERT	Pistachio, USPTO	classification	classification, reaction representation learning
RXNMapper (Schwaller et al., 2021a)	Molecule	770K	~ALBERT	USPTO	MLM	atom-mapping
MoLFormer (Ross et al., 2022)	Molecule	47M	linear attention	PubChem, ZINC	MLM	classification, regression
Chemformer (Irwin et al., 2022)	Molecule	45M, 230M	~BART	USPTO, ChEMBL, MoleculeNet	sequence to sequence, regression	regression, reaction prediction, retrosynthesis, molecule generation
R-MAT (Maziarka et al., 2024)	Molecule	–	~BERT	ZINC, ChEMBL	masked node prediction, regression	classification, regression
MolGPT (Bagal et al., 2022)	Molecule	6M	~GPT-1	ZINC, ChEMBL	next token prediction	molecule generation
T5Chem (Lu and Zhang, 2022)	Molecule	–	~T5	PubChem	sequence to sequence	classification, regression, reaction prediction, retrosynthesis
ChemGPT (Frey et al., 2023)	Molecule	4.7M, 19M, 1.2B	~GPT-Neo	PubChem	next token prediction	–
Uni-Mol (Zhou et al., 2023)	Molecule	–	SE(3) Transformer	ZINC, ChEMBL, RCSB PDB	3D position recovery	classification, regression, molecule conformation generation, binding pose prediction
TransPolymer (Xu et al., 2023a)	Molecule	–	~RoBERTa	PI1M	MLM	regression
polyBERT (Kuenneth and Ramprasad, 2023)	Molecule	86M	DeBERTa	density functional theory, experiments	MLM, regression	regression
MFBERT (Abdel-Aty and Gould, 2022)	Molecule	–	~RoBERTa	GDB-13, ZINC, PubChem, ChEMBL, USPTO	MLM	classification, regression, virtual screening
SPMM (Chang and Ye, 2024)	Molecule	–	~BERT	PubChem	next token prediction, SMILES-property matching	classification, regression, reaction prediction, retrosynthesis, SMILES-to-property generation, property-to-SMILES generation
BARTSmiles (Chilingaryan et al., 2024)	Molecule	406M	BART	ZINC	sequence to sequence	classification, regression, reaction prediction, retrosynthesis
MolGen (Fang et al., 2024b)	Molecule	406M 7B	BART LLaMA	ZINC, NPASS	sequence to sequence, prefix tuning	molecule generation
SELFormer (Yüksel et al., 2023)	Molecule	58M, 87M	~RoBERTa	ChEMBL	MLM	classification, regression
PolyNC (Qiu et al., 2024a)	Molecule	220M	T5	density functional theory, experiments	sequence to sequence	classification, regression

Table A5: Summary of LLMs in biology and medicine. “Multi”: Multiomics (*e.g.,* single-cell); “NLI”: natural language inference; “VQA”: visual question answering; “EHR”: electronic health record; “EMR”: electronic medical record; “PPI”: protein-protein interaction. Other notations have the same meaning as in previous tables.

Model	Modality	Size	Architecture	Pre-training Data	Pre-training Task(s)	Evaluation Task(s)
BioBERT (Lee et al., 2020)	L	110M, 340M	BERT	PubMed, PMC	MLM, NSP	NER, RE, QA
BioELMo (Jin et al., 2019)	L	93M	ELMo	PubMed	next token prediction, previous token prediction	NER, NLI
ClinicalBERT (Alsentzer et al., 2019)	L	110M	BERT	MIMIC-III	MLM, NSP	NER, NLI
ClinicalBERT (Huang et al., 2019)	L	110M	BERT	MIMIC-III	next token prediction, previous token prediction	word similarity estimation, hospital readmission prediction
BlueBERT (Peng et al., 2019)	L	110M, 340M	BERT	PubMed, MIMIC-III	MLM, NSP	NER, RE, NLI, classification, sentence similarity estimation
BEHRT (Li et al., 2020)	L	–	∼BERT	Clinical Practice Research Datalink	MLM	disease prediction
EhrBERT (Li et al., 2019)	L	–	∼BERT	MADE 1.0	entity linking	entity linking
Clinical XLNet (Huang et al., 2020)	L	110M	XLNet	MIMIC-III	permutation language modeling	mortality prediction
ouBioBERT (Wada et al., 2020)	L	110M	BERT	PubMed	MLM, NSP	NER, RE, NLI, classification, sentence similarity estimation
COVID-Twitter-BERT (Müller et al., 2023)	L	340M	BERT	COVID-19 tweets	MLM, NSP	classification, sentiment analysis, stance prediction
Med-BERT (Rasmy et al., 2021)	L	–	∼BERT	Cerner Health Facts	MLM, classification	disease prediction
Bio-ELECTRA (Ozyurt, 2020)	L	110M	ELECTRA	PubMed	MLM, replaced token detection	NER, QA
BiomedBERT (Gu et al., 2021)	L	110M, 340M	BERT	PubMed, PMC	MLM, NSP	NER, RE, QA, classification, sentence similarity estimation
MCBERT (Zhang et al., 2020)	L	110M	BERT	Chinese media, encyclopedia, EHRs	MLM, NSP	NER, QA, classification, retrieval, paraphrase identification
BRLTM (Meng et al., 2021a)	L	–	∼BERT	EHRs	MLM	disease prediction
BioRedditBERT (Basaldella et al., 2020)	L	110M	BERT	Reddit	entity linking	entity linking
BioMegatron (Shin et al., 2020)	L	345M	BERT	PubMed, PMC	MLM, NSP	NER, RE, QA
SapBERT (Liu et al., 2021b)	L	110M	BERT	UMLS	synonym alignment	entity linking
ClinicalTransformer (Yang et al., 2020)	L	110M 125M 12M 110M 110M 149M 86M	BERT RoBERTa ALBERT ELECTRA XLNet Longformer DeBERTa	MIMIC-III	MLM, NSP, sentence order prediction, replaced token detection, permutation language modeling	NER
BioRoBERTa (Lewis et al., 2020b)	L	125M, 355M	RoBERTa	PubMed, PMC, MIMIC-III	MLM	NER, RE, NLI, classification
RAD-BERT (Bressem et al., 2020)	L	110M	BERT	radiology reports	MLM, NSP	classification
BioMedBERT (Chakraborty et al., 2020)	L	340M	BERT	BREATHE	MLM, NSP	NER, RE, QA, retrieval
LBERT (Warikoo et al., 2021)	L	–	∼BERT	PubMed	RE	RE
ELECTRAMed (Miolo et al., 2021)	L	110M	ELECTRA	PubMed	MLM, replaced token detection	NER, RE, QA
KeBioLM (Yuan et al., 2021)	L	110M	BERT	PubMed, UMLS	MLM, NER, entity linking	NER, RE, knowledge probing
SciFive (Phan et al., 2021)	L	220M, 770M	T5	PubMed, PMC	sequence to sequence	NER, RE, QA, NLI, classification
BioALBERT (Naseem et al., 2022)	L	12M, 18M	ALBERT	PubMed, PMC, MIMIC-III	MLM, sentence order prediction	NER, RE, QA, NLI, classification, sentence similarity estimation
Clinical-Longformer (Li et al., 2022a)	L	149M 110M	Longformer BigBird	MIMIC-III	MLM	NER, QA, NLI, classification
BioBART (Yuan et al., 2022a)	L	140M, 406M	BART	PubMed	sequence to sequence	NER, entity linking, summarization, dialogue
BioGPT (Luo et al., 2022)	L	355M, 1.5B	GPT-2	PubMed	next token prediction	RE, QA, classification, generation
Med-PaLM (Singhal et al., 2023a)	L	8B, 62B, 540B	PaLM	instructions	instruction tuning	QA
GatorTron (Yang et al., 2022b)	L	345M, 3.9B, 8.9B	BERT	Wikipedia, PubMed, PMC, MIMIC-III, clinical narratives	MLM	NER, RE, QA, NLI, sentence similarity estimation
ChatDoctor (Li et al., 2023e)	L	7B	LLaMA	HealthCareMagic	instruction tuning	dialogue
DoctorGLM (Xiong et al., 2023)	L	6B	ChatGLM	medical dialogues	instruction tuning	dialogue
BenTsao (Wang et al., 2023d)	L	7B	LLaMA	instructions	instruction tuning	QA, dialogue
MedAlpaca (Han et al., 2023)	L	7B, 13B	LLaMA	medical flash cards, Stack Exchange, WikiDoc	instruction tuning	QA
PMC-LLaMA (Wu et al., 2024)	L	7B, 13B	LLaMA	biomedical papers, books, instructions	next token prediction, instruction tuning	QA
Med-PaLM 2 (Singhal et al., 2023b)	L	8B, 62B, 540B	PaLM 2	instructions	instruction tuning	QA
HuatuoGPT (Zhang et al., 2023b)	L	7B, 13B	BLOOM	instructions	instruction tuning	QA, dialogue
MedCPT (Jin et al., 2023c)	L	110M	BERT	PubMed search logs	retrieval	classification, link prediction, recommendation, retrieval, sentence similarity estimation
Zhongjing (Yang et al., 2024b)	L	13B	Ziya-LLaMA	textbooks, QA pairs, knowledge bases, EHRs, EMRs, clinical reports, instructions	next token prediction, instruction tuning	QA
DISC-MedLLM (Bao et al., 2023)	L	13B	Baichuan	instructions	instruction tuning	QA, dialogue
DRG-LLaMA (Wang et al., 2024a)	L	7B, 13B	LLaMA	MIMIC-IV	classification	diagnosis-related group prediction
Qilin-Med (Ye et al., 2023b)	L	7B	Baichuan	ChiMed-CPT, ChiMed-SFT, ChiMed-DPO	next token prediction, instruction tuning	QA, dialogue
AlpaCare (Zhang et al., 2023d)	L	7B, 13B 7B, 13B	LLaMA LLaMA-2	MedInstruct-52k	instruction tuning	QA, summarization
BianQue (Chen et al., 2023d)	L	6B	ChatGLM	BianQueCorpus	instruction tuning	dialogue
HuatuoGPT-II (Chen et al., 2023a)	L	7B, 13B, 34B	Baichuan 2	instructions	instruction tuning	QA, dialogue
Taiyi (Luo et al., 2024)	L	7B	Qwen	instructions	instruction tuning	NER, RE, QA, classification
MEDITRON (Chen et al., 2023e)	L	7B, 70B	LLaMA-2	GAP-Replay	next token prediction, instruction tuning	QA
PLLaMa (Yang et al., 2024c)	L	7B, 13B	LLaMA-2	plant science journals, instructions	next token prediction, instruction tuning	QA
BioMistral (Labrak et al., 2024)	L	7B	Mistral	PMC	next token prediction	QA
Me LLaMA (Xie et al., 2024)	L	13B, 70B	LLaMA-2	PubMed, PMC, MIMIC-III, MIMIC-IV, MIMIC-CXR, RedPajama, instructions	next token prediction, instruction tuning	NER, RE, QA, NLI, classification, summarization
BiMediX (Pieri et al., 2024)	L	8×7B	Mixtral	BiMed1.3M	instruction tuning	QA

(Biology and Medicine, Table Continued)

Model	Modality	Size	Architecture	Pre-training Data	Pre-training Task(s)	Evaluation Task(s)
MMedLM (Qiu et al., 2024b)	L	7B 1.8B, 7B 8B	InternLM InternLM2 LLaMA-3	MMedC	next token prediction	QA
BioMedLM (Bolton et al., 2024)	L	2.7B	∼GPT-2	PubMed, PMC	next token prediction	QA
Hippocrates (Acikgoz et al., 2024)	L	7B 7B	LLaMA-2 Mistral	PubMed, PMC, medical guidelines, instructions	next token prediction, instruction tuning	QA
BMRetriever (Xu et al., 2024)	L	410M, 1B 2B 7B	Pythia Gemma Mistral	biomedical papers, textbooks, QA pairs, instructions	contrastive learning, instruction tuning	QA, recommendation, retrieval, entity linking, sentence similarity estimation
Panacea (Lin et al., 2024a)	L	7B	Mistral	TrialAlign, TrialInstruct	next token prediction, instruction tuning	summarization, query generation, query expansion, trial design, patient-trial matching
G-BERT (Shang et al., 2019)	L+G	–	BERT + GAT	MIMIC-III, ICD-9, ATC	MLM, diagnosis prediction, medication prediction	medication recommendation
CODER (Yuan et al., 2022b)	L+G	110M	BERT	UMLS	link prediction	entity linking, link prediction, entity similarity estimation
MoP (Meng et al., 2021b)	L+G	–	Adapters	UMLS	link prediction	QA, NLI, classification
BioLinkBERT (Yasunaga et al., 2022b)	L+G	110M, 340M	BERT	PubMed	MLM, link prediction	NER, RE, QA, classification, sentence similarity estimation
DRAGON (Yasunaga et al., 2022a)	L+G	360M	∼BERT + ∼GAT	PubMed, UMLS	MLM, link prediction	QA
ConVIRT (Zhang et al., 2022)	L+V	–	BERT + ResNet	MIMIC-CXR, musculoskeletal text-image pairs	text-image matching	classification, text-to-image retrieval, image-to-image retrieval
MMBERT (Khare et al., 2021)	L+V	–	BERT + ResNet	ROCO	MLM	VQA
MedViLL (Moon et al., 2022)	L+V	–	BERT + ResNet	MIMIC-CXR	MLM, text-image matching	VQA, classification, text-to-image retrieval, image-to-text retrieval, report generation
GLoRIA (Huang et al., 2021)	L+V	–	BERT + ResNet	CheXpert	text-image matching	classification, segmentation, image-to-text retrieval
LoVT (Müller et al., 2022)	L+V	–	BERT + ResNet	MIMIC-CXR	text-image matching	segmentation, detection
BioViL (Boecking et al., 2022)	L+V	–	BERT + ResNet	MIMIC-CXR	MLM, text-image matching	NLI, classification, segmentation, phrase grounding
M^{3}AE (Chen et al., 2022c)	L+V	–	RoBERTa + ViT	ROCO, MedICaT	MLM, masked image modeling, text-image matching	VQA, classification, text-to-image retrieval, image-to-text retrieval
ARL (Chen et al., 2022d)	L+V	–	BERT + ViT	ROCO, MedICaT, MIMIC-CXR	MLM, masked image modeling, text-image matching	VQA, classification, text-to-image retrieval, image-to-text retrieval
CheXzero (Tiu et al., 2022)	L+V	–	Transformer + ViT	MIMIC-CXR	text-image matching	classification
MGCA (Wang et al., 2022a)	L+V	–	BERT + ResNet / ViT	MIMIC-CXR	text-image matching	classification, segmentation, detection
MedCLIP (Wang et al., 2022b)	L+V	–	BERT + Swin	MIMIC-CXR, CheXpert	text-image matching	classification, image-to-text retrieval
BioViL-T (Bannur et al., 2023)	L+V	–	BERT + ResNet	MIMIC-CXR	MLM, text-image matching	classification, report generation, sentence similarity estimation
BiomedCLIP (Zhang et al., 2023c)	L+V	–	BERT + ViT	PMC figure-caption pairs, fine-grained text-image pairs	text-image matching	VQA, classification, text-to-image retrieval, image-to-text retrieval
PMC-CLIP (Lin et al., 2023a)	L+V	–	BERT + ResNet	PMC figure-caption pairs, subfigure-subcaption pairs	MLM, text-image matching	VQA, classification, text-to-image retrieval, image-to-text retrieval
Xplainer (Pellegrini et al., 2023)	L+V	–	BERT + ResNet	MIMIC-CXR	text-image matching	classification
RGRG (Tanida et al., 2023)	L+V	–	GPT-2 + ResNet	MIMIC-CXR	detection, classification, next token prediction	report generation
BiomedGPT (Zhang et al., 2024c)	L+V	33M, 93M, 182M	∼BERT + ResNet + ∼GPT	IU X-Ray, MedICaT, PathVQA, Peir Gross, SLAKE, DeepLesion, OIA-DDR, CheXpert, CytoImageNet, ISIC, Retinal Fundus, MIMIC-III, BioNLP, PubMed	MLM, masked image modeling, object detection, VQA, image captioning	VQA, NLI, classification, summarization, image captioning, clinical trial matching, treatment suggestion, mortality prediction
Med-UniC (Wan et al., 2023)	L+V	–	BERT + ResNet / ViT	MIMIC-CXR, PadChest	text-image matching, contrastive learning	classification, segmentation, detection
LLaVA-Med (Li et al., 2023a)	L+V	7B	LLaVA	PMC figure-caption pairs, instructions	text-image matching, instruction tuning	VQA
MI-Zero (Lu et al., 2023)	L+V	–	BERT + CTransPath	histopathology figure-caption pairs	text-image matching	classification
XrayGPT (Thawkar et al., 2024)	L+V	–	LLaMA + Swin	MIMIC-CXR, Open-i	text-image matching	VQA
MONET (Kim et al., 2024)	L+V	–	BERT + ViT	PMC and textbook figure-caption pairs	text-image matching	classification, data auditing, model auditing
QuiltNet (Ikezogwo et al., 2023)	L+V	–	BERT + ViT	Quilt-1M	text-image matching	classification, text-to-image retrieval, image-to-text retrieval
MUMC (Li et al., 2023c)	L+V	–	BERT + ViT	ROCO, MedICaT, ImageCLEFmedical Caption	MLM, text-image matching	VQA
M-FLAG (Liu et al., 2023a)	L+V	–	BERT + ResNet	MIMIC-CXR	text-image matching	classification, segmentation, detection
PRIOR (Cheng et al., 2023)	L+V	–	BERT + ResNet	MIMIC-CXR	text-image matching, image reconstruction, sentence prototype generation	classification, segmentation, detection, image-to-text retrieval
Med-PaLM M (Tu et al., 2024)	L+V	12B, 84B, 562B	PaLM-E	MultiMedBench	instruction tuning	QA, VQA, classification, report generation, report summarization
CITE (Zhang et al., 2023i)	L+V	–	BERT + ViT	PatchGastric	text-image matching, prompt tuning	classification
Med-Flamingo (Moor et al., 2023)	L+V	–	Flamingo	PMC figure-caption pairs, textbooks	next token prediction	VQA
RadFM (Wu et al., 2023)	L+V	14B	LLaMA + ViT	MedMD, RadMD	next token prediction, instruction tuning	VQA, classification, report generation

(Biology and Medicine, Table Continued)

Model	Modality	Size	Architecture	Pre-training Data	Pre-training Task(s)	Evaluation Task(s)
PLIP (Huang et al., 2023)	L+V	–	GPT-2 + ViT	Twitter text-image pairs, PathLAION	text-image matching	classification, text-to-image retrieval, image-to-image retrieval
MaCo (Huang et al., 2024b)	L+V	–	BERT + ViT	MIMIC-CXR	masked image modeling, text-image matching	classification, segmentation, phrase grounding
CXR-CLIP (You et al., 2023)	L+V	–	BERT + ResNet / Swin	MIMIC-CXR, CheXpert, ChestX-ray14	text-image matching, contrastive learning	classification, image-to-text retrieval
Qilin-Med-VL (Liu et al., 2023b)	L+V	–	LLaMA-2 + ViT	ChiMed-VL-Alignment, ChiMed-VL-Instruction	text-image matching, instruction tuning	VQA
BioCLIP (Stevens et al., 2024)	L+V	–	GPT-2 + ViT	TreeOfLife-10M	text-image matching	classification
M3D (Bai et al., 2024)	L+V	–	LLaMA-2 + ViT	M3D-Cap, M3D-VQA, M3D-RefSeg, M3D-Seg	text-image matching, instruction tuning	VQA, segmentation, text-to-image retrieval, image-to-text retrieval, report generation, 3D positioning
Med-Gemini (Saab et al., 2024)	L+V	–	Gemini	MedQA, LiveQA, HealthSearchQA, MedicationQA, MIMIC-III, SLAKE, PathVQA, ROCO, PAD-UFES-20, MIMIC-CXR, ECG-QA	instruction tuning	QA, VQA, signal QA, video QA, classification, long-form text generation, long EHR understanding
Med-Gemini-2D/3D/Polygenic (Yang et al., 2024a)	L+V	–	Gemini	SLAKE, MIMIC-CXR, Digital Knee X-ray, CXR-US2, NLST, CT-US1, PathVQA, Histopathology, PAD-UFES-20, EyePACS, PMC-OA, VQA-Med, UK Biobank	VQA, captioning, instruction tuning	VQA, classification, report generation, disease risk prediction
Mammo-CLIP (Ghosh et al., 2024)	L+V	–	BERT + EfficientNet	UPMC, VinDr-Mammo	text-image matching	classification, localization
ProtTrans (Elnaggar et al., 2021)	Protein	420M 224M 409M 420M 3B, 11B	∼BERT ∼ALBERT ∼XLNet ∼ELECTRA T5	UniRef50, UniRef100, BFD	MLM, permutation language modeling, replaced token detection, sequence to sequence	secondary structure prediction, function prediction
ESM-1b (Rives et al., 2021)	Protein	650M	∼BERT	UniRef50, UniRef100	MLM	secondary structure prediction, contact prediction, remote homology detection
MSA Transformer (Rao et al., 2021)	Protein	100M	∼BERT	UniRef50	MLM	secondary structure prediction, contact prediction
ESM-1v (Meier et al., 2021)	Protein	650M	∼BERT	UniRef90	MLM	mutation effect prediction
AminoBERT (Chowdhury et al., 2022)	Protein	–	∼BERT	UniParc	MLM, chunk permutation prediction	secondary structure prediction, contact prediction
ProteinBERT (Brandes et al., 2022)	Protein	16M	∼BERT	UniRef90, Gene Ontology	MLM	secondary structure prediction, remote homology detection, fitness prediction
ProtGPT2 (Ferruz et al., 2022)	Protein	738M	GPT-2	UniRef50	next token prediction	secondary structure prediction, disorder prediction, protein sequence generation
ESM-IF1 (Hsu et al., 2022)	Protein	142M	Transformer + GVP-GNN	UniRef50	next token prediction	fixed backbone protein design, mutation effect prediction
ProGen (Madani et al., 2023)	Protein	1.6B	CTRL	UniParc, UniprotKB, Pfam, NCBI Taxonomy	next token prediction	protein sequence generation
ProGen2 (Nijkamp et al., 2023)	Protein	151M, 764M, 2.7B, 6.4B	∼GPT-3	UniRef90, BFD	next token prediction	protein sequence generation, fitness prediction
ESM-2 (Lin et al., 2023b)	Protein	8M, 35M, 150M, 650M, 3B, 15B	∼BERT	UniRef50, UniRef90	MLM	secondary structure prediction, contact prediction, 3D structure prediction
Ankh (Elnaggar et al., 2023)	Protein	450M, 1.1B	∼T5	UniRef50	sequence to sequence	secondary structure prediction, contact prediction, embedding-based annotation transfer, remote homology detection, fitness prediction, localization prediction
ProtST (Xu et al., 2023b)	Protein	–	∼BERT	Swiss-Prot	MLM, text-protein matching	fitness prediction, localization prediction, function annotation
LM-Design (Zheng et al., 2023b)	Protein	659M	∼BERT + ProtMPNN	CATH, UniRef50	MLM	fixed backbone protein design
ProteinDT (Liu et al., 2023c)	Protein	–	∼BERT	Swiss-Prot	text-protein matching	text-to-protein generation, text-guided protein editing, secondary structure prediction, contact prediction, remote homology detection, fitness prediction
Prot2Text (Abdine et al., 2024)	Protein	256M, 283M, 398M, 898M	∼BERT + R-GCN + ∼GPT-2	Swiss-Prot	sequence to sequence	protein-to-text generation
BioMedGPT (Luo et al., 2023c)	Protein	10B	LLaMA-2 + GraphMVP + ESM-2	S2ORC, PubChemQA, UniProtQA	next token prediction, instruction tuning	QA
SaProt (Su et al., 2024)	Protein	35M, 650M	∼BERT	UniRef50	MLM	mutation effect prediction, fitness prediction, localization prediction, function annotation, PPI prediction
BioT5 (Pei et al., 2023)	Protein	220M	T5	C4, ZINC, UniRef50, PubMed, PubChem, Swiss-Prot	sequence to sequence	molecule property prediction, protein property prediction, drug-target interaction prediction, PPI prediction, molecule captioning, text-based molecule design
ProLLaMA (Lv et al., 2024)	Protein	7B	LLaMA-2	UniRef50, instructions	next token prediction, instruction tuning	protein sequence generation, protein property prediction

(Biology and Medicine, Table Continued)

Model	Modality	Size	Architecture	Pre-training Data	Pre-training Task(s)	Evaluation Task(s)
DNABERT (Ji et al., 2021)	DNA	110M	BERT	GRCh38	MLM	chromatin profile prediction, promoter prediction, splice site prediction, functional genetic variant identification
GenSLMs (Zvyagin et al., 2023)	DNA	25M, 250M, 2.5B, 25B	∼GPT-2	prokaryotic gene sequences	next token prediction	SARS-CoV-2 genome evolution prediction
Nucleotide Transformer (Dalla-Torre et al., 2023)	DNA	50M, 100M, 250M, 500M	∼BERT	GRCh38, 1000 Genomes, multispecies genomes	MLM	chromatin profile prediction, enhancer prediction, promoter prediction, epigenetic marks prediction, splice site prediction
GENA-LM (Fishman et al., 2023)	DNA	110M, 340M 110M	BERT BigBird	T2T-CHM13, 1000 Genomes, multispecies genomes	MLM	enhancer prediction, promoter prediction, epigenetic marks prediction, splice site prediction, species classification
DNABERT-2 (Zhou et al., 2024a)	DNA	110M	BERT	GRCh38, multispecies genomes	MLM	chromatin profile prediction, promoter prediction, epigenetic marks prediction, splice site prediction, species classification, SARS-CoV-2 variant prediction, enhancer-promoter interaction
HyenaDNA (Nguyen et al., 2023a)	DNA	0.4M, 3.3M, 6.6M	Hyena	GRCh38	next token prediction	chromatin profile prediction, enhancer prediction, promoter prediction, epigenetic marks prediction, splice site prediction, species classification
DNAGPT (Zhang et al., 2023a)	DNA	0.1B, 3B 6.6M	∼GPT-3	Ensembl	next token prediction, sequence order prediction, regression	genome generation, chromatin profile prediction, promoter prediction, genomic signals and regions recognition
RNABERT (Akiyama and Sakakibara, 2022)	RNA	–	∼BERT	RNAcentral	MLM	RNA structural alignment, RNA clustering
RNA-FM (Chen et al., 2022b)	RNA	–	∼BERT	RNAcentral	MLM	secondary structure prediction, 3D structure prediction, protein-RNA interaction, mean ribosome load prediction
SpliceBERT (Chen et al., 2024)	RNA	19.4M	∼BERT	UCSC genome browser	MLM	human branchpoint prediction, splice site prediction
RNA-MSM (Zhang et al., 2024g)	RNA	–	∼BERT	Rfam	MLM	secondary structure prediction, solvent accessibility prediction
CodonBERT (Li et al., 2023d)	RNA	–	∼BERT	mRNA sequences	MLM, homologous sequences prediction	mRNA property prediction
UTR-LM (Chu et al., 2024)	RNA	–	∼BERT	5' UTR sequences	MLM, classification, regression	mean ribosome load prediction, mRNA property prediction, internal ribosome entry site prediction
scBERT (Yang et al., 2022a)	Multi	–	Performer	PanglaoDB	MLM	cell type annotation, novel cell type discovery
scGPT (Cui et al., 2024)	Multi	–	∼GPT-3	CELLxGENE	MLM	cell type annotation, perturbation response prediction, multi-batch integration, multi-omic integration, gene network inference
scFoundation (Hao et al., 2024)	Multi	100M	Transformer + Performer	scRNA-seq data	MLM	cell clustering, drug response prediction, perturbation response prediction, cell type annotation, gene network inference
Geneformer (Theodoris et al., 2023)	Multi	10M, 40M	∼BERT	Genecorpus-30M	MLM	gene dosage sensitivity prediction, chromatin dynamics prediction, network dynamics prediction
CellLM (Zhao et al., 2023b)	Multi	–	Performer	PanglaoDB, CancerSCEM	MLM, classification, contrastive learning	cell type annotation, drug sensitivity prediction
CellPLM (Wen et al., 2024)	Multi	82M	Transformer	scRNA-seq data, spatially-resolved transcriptomic data	MLM	cell clustering, scRNA-seq denoising, spatial transcriptomic imputation, cell type annotation

Table A6: Summary of LLMs in geography, geology, and environmental science. "Climate": Climate Time Series; "POI": point of interest. Other notations have the same meaning as in previous tables.

Model	Modality	Size	Architecture	Pre-training Data	Pre-training Task(s)	Evaluation Task(s)
ClimateBERT (Webersinke et al., 2021)	L	82M	DistilRoBERTa	climate-related news, papers, corporate climate reports	MLM	classification, fact-checking
SpaBERT (Li et al., 2022b)	L	110M, 340M	BERT	OpenStreetMap	MLM, masked entity prediction	entity typing, entity linking
MGeo (Ding et al., 2023)	L	213M	∼BERT	text-geolocation pairs	MLM, masked geographic modeling, contrastive learning	query-POI matching
K2 (Deng et al., 2024)	L	7B	LLaMA	geoscience papers, Wikipedia, instructions	next token prediction, instruction tuning	QA
OceanGPT (Bi et al., 2023b)	L	7B	LLaMA-2	ocean science papers, instructions	next token prediction, instruction tuning	QA, classification, extraction, knowledge probing, commonsense reasoning, summarization, generation

(Geography, Geology, and Environmental Science, Table Continued)

Model	**Modality**	**Size**	**Architecture**	**Pre-training Data**	**Pre-training Task(s)**	**Evaluation Task(s)**
ClimateBERT-NetZero (Schimanski et al., 2023)	L	82M	DistilRoBERTa	Net Zero Tracker	classification	classification
GeoLM (Li et al., 2023f)	L	110M, 340M	BERT	OpenStreetMap, Wikipedia	MLM, contrastive learning	NER, RE, entity typing, entity linking
GeoGalactica (Lin et al., 2024c)	L	30B	Galactica	geoscience papers, code, Wikipedia, instructions	next token prediction, instruction tuning	QA, knowledge probing, quantitative reasoning, summarization, generation
ERNIE-GeoL (Huang et al., 2022)	L+G	–	Transformer + graph aggregation	Baidu Maps (POI database, search logs)	MLM, geocoding	classification, query-POI matching, address parsing, geocoding, next POI recommendation
PK-Chat (Deng et al., 2023)	L+G	132M	∼UniLM	Geoscience Academic Knowledge Graph	next token prediction, bag-of-words prediction, classification	task-oriented dialogue
UrbanCLIP (Yan et al., 2024)	L+V	–	Transformer + ViT	satellite images, location descriptions,	next token prediction, text-image matching	urban indicator prediction
FourCastNet (Pathak et al., 2022)	Climate	–	∼ViT	ERA5	regression	weather forecasting
Pangu-Weather (Bi et al., 2023a)	Climate	–	∼Swin	ERA5	regression	weather forecasting
ClimaX (Nguyen et al., 2023c)	Climate	–	∼ViT	CMIP6	regression	weather forecasting, climate projection, climate model downscaling
FengWu (Chen et al., 2023b)	Climate	–	Transformer	ERA5	regression	weather forecasting
W-MAE (Man et al., 2023)	Climate	–	ViT	ERA5	masked image modeling	weather forecasting
FuXi (Chen et al., 2023c)	Climate	–	∼Swin V2	ERA5	regression	weather forecasting