

Language + Molecules

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1 Description

Climate change, access to food and water, pandemics—these words, when uttered, immediately summon to mind global challenges with possible disastrous outcomes. The world faces enormous problems in the coming decades on scales of complexity never-before-seen. To address these issues, developing scientific solutions which are scalable, flexible, and inexpensive is critical. Further, we need to develop these solutions quickly. Broadly speaking, chemistry can provide molecular solutions to many of these problems: breakthrough drugs (e.g., kinase inhibitors (Ferguson and Gray, 2018)), materials (e.g., organic photovoltaics (Kippelen et al., 2009)), and chemical processes. The extremely large search spaces in which these solutions exist make AI tools critical for finding them. Of particular note, multimodal models combining language with molecules are poised to be a critical tool for discovering these solutions (Zhang et al., 2023). In this tutorial, we will discuss the role which natural language processing can play in discovering and accelerating solutions to global problems via the broad chemistry domain.

One of the first questions that probably comes to mind is why we would want to integrate natural language with molecules. Succinctly, combining these types of information has the possibility to accelerate scientific discovery. As motivating scenarios, imagine a future where a doctor can receive a novel, patient-specific drug necessary to treat an ailment just by writing a few sentences describing the patient’s symptoms (also taking into account their genotype, phenotype, and medical history). Or, imagine a scientist tackling challenging problems by designing a molecule satisfying desired functions (e.g., antimalarial or a photovoltaic) rather than its structure or low level properties (e.g., solubility). Controlling molecules and drug design in such a high-level manner has potential to be hugely impactful, but it requires a method of abstract de-

scription; luckily, humans have already developed one: natural language.

In recent months, because of this potential impact, significant attention and growth has occurred in scientific NLP and AI research, including integration of molecules with natural language and multimodal AI for science/medicine ((Zhang et al., 2023) Section 10.3.3, (Wang et al., 2023)). We believe a sufficient amount of work has now been done, along with significant interest generated, to propose an **Introductory to NLP** (yet still **Cutting-Edge**) tutorial on "Language + Molecules". This tutorial is designed to require no knowledge and will enable participants to begin exploring relevant and impactful research. Since most relevant work is still cutting-edge, this will broaden the community’s understanding of the associated challenges, methodologies, and goals in multimodal molecule-language models. We will present an interactive hands-on example and release accompanying relevant code and resources. The tutorial will precede and prepare the way for the Language+Molecules workshop later in the year at ACL.

2 Outline [180 min.]

Applying language models to the scientific domain is becoming increasingly popular due to its potential impact for accelerating scientific discovery (Hope et al., 2022). Beyond extracting information from scientific literature, NLP has the possibility to increase control of the scientific discovery process, which can be achieved through multimodal representations and generative language models.

2.1 Background [60 min.]

Scientific Information Extraction [15 min.]

To start, we will provide a high-level overview on traditional NLP tasks used for scientific discovery (e.g., named entity recognition, entity linking, and relation extraction), as well as recent domain-specific LLMs designed for superior performance

on scientific tasks (Beltagy et al., 2019).

What is a molecule? [15 min.]

Half of the title is molecules, but what is one? We will start from scratch and discuss what a molecule actually is, including the basic constituents of molecules, atoms and bonds, and how they essentially form graph structures. Then, we will focus on molecular string languages, which are a key building block for chemical language models. We will discuss tradeoffs of these languages (Grisoni, 2023; Weininger, 1988; O’Boyle and Dalke, 2018; Krenn et al., 2020; Cheng et al., 2023). Krenn et al. (2020) proposes a formal grammar approach, which may particularly interest the ACL community.

Molecule Design using Language Models [15]

Now that we know what a molecule is, we will overview recent work applying NLP techniques to these molecular languages with impressive results. These molecular LLMs are trained with adapted pre-training techniques from (natural) language models to learn molecule representation from large collections of molecule strings (Frey et al., 2022; Chithrananda et al., 2020; Ahmad et al., 2022; Fabian et al., 2020; Schwaller et al., 2021; NVIDIA Corporation, 2022; Flam-Shepherd and Aspuru-Guzik, 2023; Tysinger et al., 2023). Applications include molecule and material generation, property prediction, and protein binding site prediction.

Drug Discovery—A Brief Primer [15 min.]

Ok, so NLP is being used for molecules now. What can we do with it?—here, we present a brief overview of drug discovery—an important but challenging problem. Historically, molecular discovery has commonly been done by humans who design and build individual molecules, but this can cost over a billion dollars and take over ten years (Gaudelet et al., 2021). We’ll discuss a little of the process here, including non-NLP deep learning methods, so that we know how to improve it.

2.2 Integrating Language with Molecules [95]

What does natural language have to offer? [15]

At least at first, integrating languages and molecules seems like an odd idea. Here, we’ll start an interactive discussion with the audience on what they think potential benefits might be. We’ll make sure to mention the following major advantages, as discussed in the recent survey (Zhang et al., 2023):

1. **Generative Modeling:** One of the largest problems in current LLMs—hallucination—becomes a strength for discovering molecules with high-level functions and abstract properties. In particular, language is compositional by nature (Szabó, 2020; Partee et al., 1984; Han et al., 2023), and therefore holds promise for composing these high-level properties (e.g., antimalarial) (Liu et al., 2022).
2. **Bridging Modalities:** Language can serve to “bridge” between modalities for scarce data.
3. **Domain Understanding:** Grounding language models into external real world knowledge (here, molecular structures) can improve understanding of unseen molecules and advance many emerging tasks, such as experimental procedure planning, which use LLMs as scientific agents.
4. **Democratization:** Language enables scientists without computational expertise to leverage advances in scientific AI.

Do I want multimodality? [5 min.]

An important, yet often overlooked, question in multimodal NLP is to ask: do I need multimodality? For example, if one wants to extract reactions from the literature, a text-to-text model (Vaucher et al., 2020) might be sufficient. However, editing a drug with high-level instructions requires language (Liu et al., 2023a; Fang et al., 2023). Here, we will dive into this question and discuss example scenarios with the audience for how to answer it.

2.2.1 Integrating Modalities [30 min.]

Ok, we’ve decided we want or need multimodality. Next, we need to discuss how people are currently tackling this—we’ll start with two primary methods, bi-encoder models and joint representation models.

Bi-Encoder Models (and beyond) Bi-encoder models consist of an encoder branch for text and a branch for molecules. They have the advantage of not requiring direct, early integration of the two modalities, allowing existing single-modal models to be integrated. Representative examples we will discuss include Text2Mol (Edwards et al., 2021), CLAMP (Seidl et al., 2023), and BioTranslator (Xu et al., 2023). Generally, bi-encoder models are effective for cross-modal retrieval (Edwards et al., 2021; Su et al., 2022; Liu et al., 2022; Zhao et al., 2023b), but they may also be integrated into molecule (Su et al., 2022; Liu et al., 2022) and protein (Liu et al., 2023b) generation frameworks.

We'll talk about all these tasks, applications, and return to some important motivations (e.g., bridging modalities).

Joint Molecule-Language Models Joint models, on the other hand, seeks to model interactions between multiple modalities inside the same network to allow fine-grained interaction. We will discuss encoder-only models (Zeng et al., 2022), encoder-decoder models (Christofidellis et al., 2023), and decoder-only models (Liu et al., 2023c).

Model Differences: We will answer important questions such as: Which model should I use? What tasks can each do? Tasks include retrieval (Edwards et al., 2021), "translation" between molecules and language (Edwards et al., 2022a), editing molecules (Liu et al., 2022), and chemical reaction planning (Vaucher et al., 2020, 2021).

An Interactive Example - Targeting Microtubules for Cancer Treatment [20 min.]

At this point, there's been a lot of ideas thrown around. We'll consolidate them by exploring an interactive example of language-enabled molecule design using Google Colab.

We will focus on microtubules for the example. These cellular structures play an important role in many processes such cell growth and division, and mutations can be oncogenic (Mukhtar et al., 2014; Wattanathamsan and Pongrakhananon, 2022). In modern medicine, tumors such as pancreatic cancer are commonly treated by microtubule-targeting drugs such as paclitaxel (Albahde et al., 2021). In our example, we will explore creating new drugs with this function using natural language instructions, which may be useful in cases of paclitaxel resistance (Kavallaris, 2010). Our hands-on example will consist of three components:

1. Language-enabled Drug Design:

Participants will explore inputs to language→molecule models to generate candidate drugs which target microtubules.

2. Language-Guided Assay Testing:

Here, participants will test their proposed drugs in an assay. We will follow (Seidl et al., 2023), where natural language descriptions are used for assay predictions.

3. Interaction Prediction:

Finally, we will test if proposed drugs bind with beta-tubulin using Autodock Vina, a well established docking program (Trott and Olson, 2010), via DockString (García-Ortegón et al., 2022).

Applications [25 min.] Here, we will discuss important applications to improve cross-discipline communication, including drug discovery (Mukhtar et al., 2014; Ferguson and Gray, 2018), organic photovoltaics (Kippelen et al., 2009), and catalyst discovery for renewable energy (Zitnick et al., 2020).

2.3 Recent Trends and Conclusion [25 min.]

Instruction-Following Molecular Design [10]

In the last year, instruction-following language models (Wei et al., 2021) have surged in popularity. Following this trend, training methodologies and datasets have recently emerged to allow language models to follow instructions related to molecule properties (Liang et al., 2023; Fang et al., 2023; Zeng et al., 2023; Zhao et al., 2023a). We will give a brief overview of this new line of work.

LLMs as Scientific Agents [5 min.] Further, we'll focus on recent work which looks to control experiments with language models (Boiko et al., 2023) and to create tools for enabling domain-specific capabilities in general language models (Bran et al., 2023; Liu et al., 2023a).

Conclusion [10 min.] We will discuss the key difficulties in the molecule-language domain that need to be addressed by the research community to allow similar progress to the vision-language domain. This includes 1) data scarcity due to domain expertise requirements, 2) addressing inconsistency when training on scientific literature, 3) improved methods for integrating geometric structures into LLMs, and 4) developing better evaluation metrics for chemical predictions without real-world experiments.

3 Logistics and Details

Diversity Considerations For this tutorial, our team originates from geographically distant countries and has varying level of seniority, including two PhD students and a full professor. The team includes a female researcher. This tutorial will augment a workshop on "Language + Molecules" to be held at the ACL conference, which already has confirmed speakers and organizers with diversity in geography, ethnicity, and gender. This tutorial will strongly promote academic diversity, since it requires combining the specialties of chemists, physicians, pharmacists, computational linguists, and machine learning researchers. Further, this tutorial will promote the usage of NLP in high-impact

areas, ranging from drug discovery to organic photovoltaics. The methods we will introduce are language-agnostic. All tutorial materials (slides, example, reading list) will be shared to reach such a diverse audience.

Target Audience and Background We will target this tutorial at NLP researchers with no knowledge of chemistry or molecules—thus, we will provide an extensive discussion of background material. However, we will assume that the target audience is familiar with modern NLP methods including training deep neural network-based language models (e.g., BERT). We anticipate an audience size of 75-150 researchers. We will discuss relevant background for applying NLP to molecules and important applications in chemistry.

Reading List

- Molecule Representations and Language Models: (Weininger, 1988; Krenn et al., 2020; Cheng et al., 2023; Chithrananda et al., 2020; Ahmad et al., 2022; Tysinger et al., 2023)
- Molecule-Language Modeling: (Edwards et al., 2021; Zhao et al., 2023b; Zeng et al., 2022; Edwards et al., 2022b; Zhao et al., 2023a; Su et al., 2022; Liu et al., 2022, 2023c; Xu et al., 2023; Liu et al., 2023a; Luo et al., 2023)
- Applications: (Jordan and Roughley, 2009; Mukhtar et al., 2014; Kippelen et al., 2009)
- LLMs as Scientific Agents: (Boiko et al., 2023; Bran et al., 2023; Castro Nascimento and Pimentel, 2023; White et al., 2023)
- Survey: (Zhang et al., 2023) Section 10.3.3

We won’t require reading these beforehand to ensure the tutorial is introductory.

Breadth of Tutorial Papers in the reading list were created by a diverse set of authors and include other disciplines. Specifically, only 2 papers and a survey from the instructors will be covered.

Ethical Considerations

Broader Impacts Our tutorial will have potential broader impacts: 1) It will help ACL researchers to better understand the research goals and constraints in chemical sciences, allowing them to do more impactful research there. 2) Studying language models in the context of non-human languages can help develop an understanding of their workings; due to our own personal linguistic biases, human researchers often misattribute abilities to language models. This is particularly relevant for developing new methodologies which are applicable to

low-resource human languages. 3) It will promote further research in text-based molecule generation, with potential to enable a large shift in chemistry research so that custom molecules can be developed for each application or patient.

Ethical Concerns Like most methodologies reliant on LLMs, there may be biases learned by the model due to its large-scale training data. In this domain, these biases may affect what type of molecules are generated. Thus, any molecules or drugs discovered should be strictly evaluated by standard clinical processes before being considered for human or medicinal use. Another risk is that potentially dangerous molecules may be discovered. However, knowledge of dangerous molecule’s existence and structure is generally not harmful due to the requisite technical knowledge and laboratory resources required for synthesis. Overall, we believe these downsides are outweighed by the benefits to the research and pharmaceutical communities.

3.1 Tutorial Presenters

Carl Edwards is a Ph.D. student in the Computer Science Department at UIUC. Broadly, he is interested in information extraction, information retrieval, text mining, representation learning, AI4Science, and multimodality. Particularly, he is interested in applying these to the scientific domain to accelerate scientific discovery. His work focuses on integrating natural language and molecules, especially using multimodal representations.

Qingyun Wang is a Ph.D. student in computer science at UIUC. His research lies in NLP for scientific discovery. Recently, he works on extracting reaction information from scientific literature. He served as a PC member in conferences including ICML, ACL, ICLR, NeurIPS, etc. His work was recognized in the first Alexa Prize competition and by the NAACL-HLT 2021 Best Demo Award. He has presented a tutorial at EMNLP 2021.

Heng Ji is a professor at the Computer Science Department of UIUC, and Amazon Scholar. She is a leading expert on multimodal multilingual information extraction, including NLP for Science with a particular interest in leveraging NLP for drug discovery. She has coordinated the NIST TAC Knowledge Base Population task since 2010. She has served as the PC Co-Chair of many conferences including NAACL-HLT2018 and ACL-IJCNLP2022 and has presented many tutorials. She was elected as NAACL secretary 2020-2023.

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