Extracting a Database of Challenges and Mitigation Strategies for Sodium-ion Battery Development

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Abstract

Sodium-ion batteries (SIBs) are emerging as a promising solution for grid-scale energy storage applications due to the widespread availability of sodium and the anticipated cost-effectiveness. The manufacturing expertise established for lithium-ion batteries (LIBs) offers a solid foundation for the development of SIBs. However, to realize their full potential, specific challenges related to the synthesis and performance of electrode materials in SIBs must be overcome. This work extracts a large database of challenges limiting the performance and synthesis of SIB cathode active materials (CAMs) and pairs these challenges with corresponding proposed mitigation strategies from the SIB literature by employing custom natural language processing (NLP) tools. The database is meant to help scientists expedite the development and exploration of SIBs.

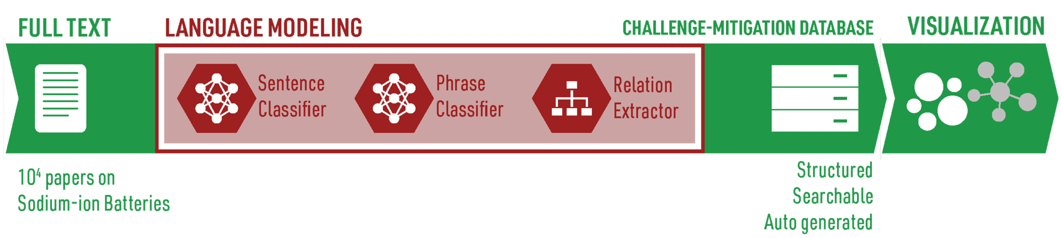

Figure 1: **NLP Pipeline**: We implemented a sequential filtering and visualization approach, employing sentence classification [1], phrase-level classification, and relationship extraction [2, 3]. The outcomes are visualized through BERT-based topic modeling [4] in Figure 3 and knowledge graphs in Figure 4.

1 Introduction

Clean energy transition is crucial to mitigating climate change [5]. Energy storage devices, particularly compact chemical energy formats like batteries, are essential for managing the intermittent nature of renewable sources like solar and wind energy [6]. LIBs are a common battery chemistry offering highest energy density and output voltage compared to alternatives [7]. However, concerns have been raised regarding the skewed geographic impact of lithium extraction and the price impact of rapid growth [8]. The development of alternative battery chemistries, such as those based on sodium, could offer diversification opportunities [9, 10, 11]. SIBs could replace LIBs for grid storage applications. While SIB fabrication can parallel that of LIBs in terms of cell manufacturing and assembly [12, 13], the commercialization of SIBs is limited by the performance of cathode active materials for SIBs [14, 15].

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Tracking scientific developments can be complex as insights across material types are buried in an enormous corpus of more than 10,000 publications [16]. Therefore, offering a coherent overview and an ability to efficiently query these insights provides value for battery researchers. NLP-based studies in materials science have focused on the extraction of quantitative synthesis-related data and materials properties, enabling training of machine learning models [17, 18, 19, 20]. This approach however, neglects text-based qualitative rationales formulated by scientists. In contrast, our methodology focuses on capturing authors' reasoning regarding structure-property relationships of performance challenges directly. These are then aligned with the relevant mitigation strategies. We believe that the intentional focus of our method on textual references to materials engineering methods and mechanisms, rather than on quantitative data can enhance the understanding of existing approaches. Our primary contributions are as follows:

- Extraction of a detailed database on SIBs materials challenges and mitigation strategies
- Interactive search tool for scientists to find SIB-related mitigation strategies and linked mechanistic causes corresponding to observed performance characteristics
- Classifiers and training data for efficient battery literature screening, extendable to LIB research

Our approach uses systematic extraction of challenges and mitigation strategies from the literature using a two-stage process of sentence and phrase extraction. Moreover, this specialized focus on SIBs, which are a critical and emerging area in battery technology, fills a specific knowledge gap in the field. The interactive search tool not only aids in research but also in practical problem-solving, allowing for a more dynamic and user-friendly way to access complex information.

2 Methods and Framework

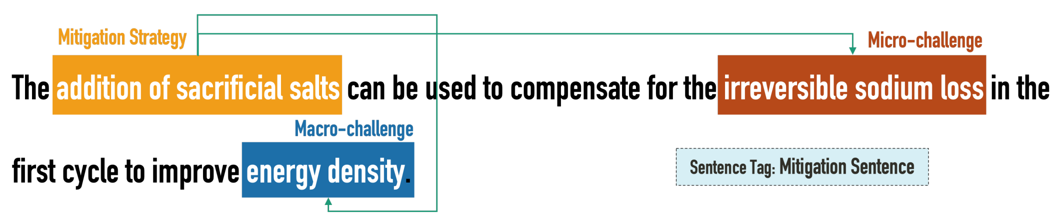

Figure 2: **Sentence, Phrase and Relationship Extraction:** After classifying the sentence to be of type "Mitigation", phrases and relationships between phrases are identified.

In recent years, there has been a surge in published research papers on SIBs to the order of 10^4 [16]. It would take over 20,000 uninterrupted hours to manually read and comprehend every single paper, assuming an average of two hours per paper. Based on our established NLP pipeline, we are able to process a corpus of 10,000 papers in 6 hours without human intervention. Our methodology builds upon seminal works in sentence-oriented sentiment analysis [21, 22, 23], sentence-based search mechanisms [1, 24], open information extraction [3, 2], and topic modeling [4].

We extracted a structured database, which enabled us to identify prominent topics from and infer implications about scalability-informed lab research. The relevant papers were downloaded using a literature mining pipeline described in [18]. We organized extracted information for 18 cathode material types across layered metal oxides, Prussian blue analogs, and polyanionics. Figure 1 illustrates the NLP pipeline tasks. Our pipeline can be used for several similar tasks. The sentence classification, phrase classification and relationship extraction methodology is described below.

Sentence Classification: We distinguish between two main types of sentences:

- **Challenge Sentences** encapsulate discussions about all performance or materials-related flaws, their mechanistic origins, and shortcomings in synthesis procedures. (e.g., *"Irreversible sodium loss in sodium-ion batteries results in low specific capacity."*)
- **Mitigation Sentences** involve references to enhancing the material's key performance indices or associated properties and methods. (e.g. in Figure 2)

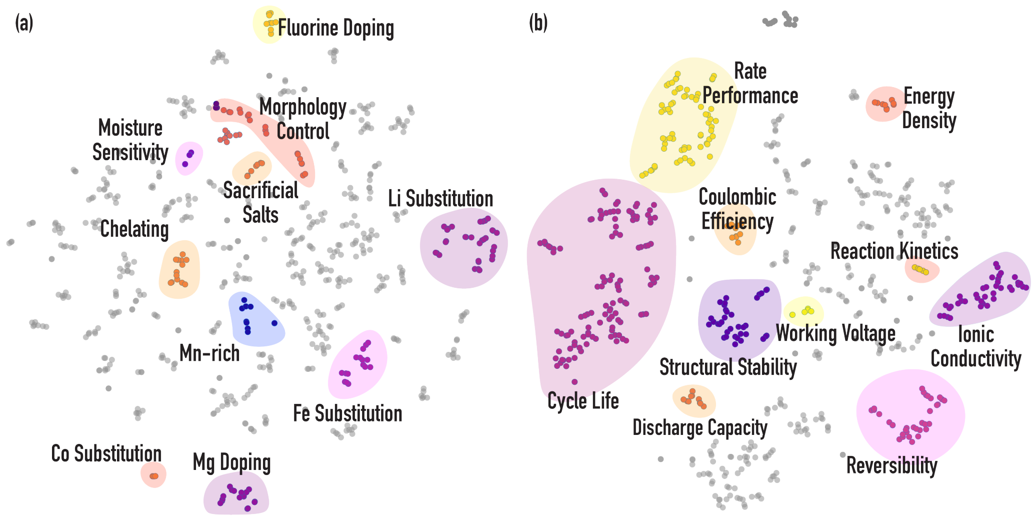

Figure 3: **Exploratory view of extracted mitigation sentences in Sodium Iron Manganese Oxide:** The extracted phrases are embedded using BERT and subsequently clustered and dimensionally reduced. *(a)* Mitigation strategy phrases with marked regions showcasing various mitigation strategy topics *(b)* Space of extracted challenge phrases. Marked regions showcase various materials related challenges.

Phrase Classification and Relationship Extraction: To extract relevant context spans from the sentences, we developed a phrase-level classification scheme. We assess challenges at two scales for phrase-level classification: macro-challenges and micro-challenges. Macro-challenges are key performance challenges directly linked to resultant performance like *"low specific capacity"*, *"poor rate capability"*., etc. whereas, micro-challenges are mechanistic causes of these macro-challenges that indicate the underlying phenomena that contribute to macro-challenges like *"low redox activity"*, *"irreversible Na loss"*, etc. Besides these two types of challenges, we extracted phrases related to mitigation strategies (e.g., *"addition of sacrificial salts"*). We also extracted the relationship among those phrases. Figure 3 visualizes the mitigation strategies space for NFMO (Sodium Iron Manganese Oxide) clustered using phrases. Extracted challenges and mitigation strategies constitute challenge-mitigation pairs.

Model Evaluation: For the development of our sentence and phrase classifiers, we benchmarked with a variety of approaches on our dataset, using stratified data splits and hyperparameter optimization. As seen in Table 1, the performance of BERT-based models [25] was commendable. The best results were attained with SciBERT [26] and MatSciBERT [27], which were both pretrained in the domain of scientific publications. We also discovered that recent autoregressive Large Language Models (LLMs), such as GPT-3 [28], yielded promising results, even when only presented with 10 in-context examples [28]. Phrase and relation extraction has been achieved with the Dynamic Graph Based Information Extraction (DyGIE) model [3].

3 Results and Discussion

Our approach enabled us to create a comprehensive database of materials-specific challenges and their mechanistic sources that impact material performance, along with corresponding mitigation strategies. In total, we obtained a database of approximately 31,000 challenge and mitigation sentences. Out of these, our classifiers identified 9,000 relations. Analyzing the diversity of papers in the final relational database, we note that 91% of the initial papers are represented in the mitigation sentence database and 84% in the challenge sentences database, underscoring the comprehensive coverage of our source material. Domain experts evaluated the informativeness and correctness of the extracted relationships which yielded a correctness score of 85%. The database can be queried for a variety of challenge-mitigation pairs using challenge topics to aid in expediting the development of commercial-scale SIBs. We clustered our mitigation database (Figure 3) using sentence BERT [29] computed embeddings of

	F1	P	R
MATSCIBERT	83.1 (1.2)	83.4 (1.1)	83.8 (1.3)
SCIBERT	**84.1 (1.7)**	**84.4 (1.5)**	**84.2 (1.4)**
GPT3 @10 SHOTS	73.2	75.9	72.5

	Sentences	Phrases	Relations
CHALLENGE	84.1	67.5	39.4
MITIGATION	83.1	67.9	50.8

Table 1: *Top:* Model comparison on the sentence classification task for challenge sentences. *Bottom:* F1 scores for sentence classification, phrase classification and relationship extraction. Our hypothesis is that the comparatively lower scores observed for Challenge relations may be attributed to the increased complexity inherent in these sentences often describing interrelated materials specific phenomena.

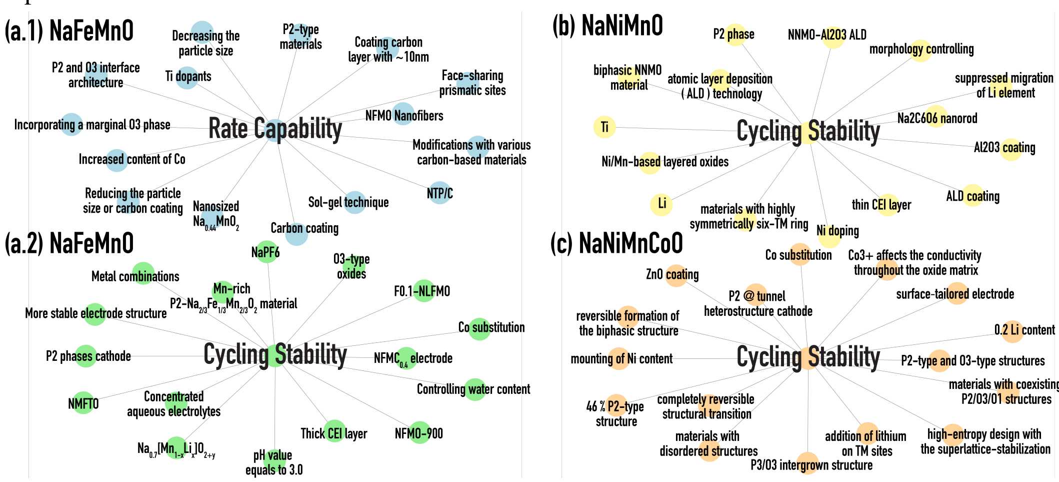

Figure 4: **Knowledge-graph representation** of some mitigation strategies linked to the macro-challenges of 'Rate Capability' and 'Cycling Stability' which are the two most commonly reported macro-challenges. These graphs were constructed by utilizing our relationship extractor to get "challenge-mitigation pairs". *(a.1)* and *(a.2)* are for NaFeMnO type materials, *(b)* is for NaNiMnO type materials and *(c)* is for NaNiMnCoO type materials.

the strategies, revealing a holistic map of the diverse mitigation strategies space. We also created knowledge graphs as shown in Figure 4 to identify "challenge-mitigation pairs" of interest.

To make the database more accessible for researchers, we integrated the large database with ChatGPT's custom GPT creator [30] to create a *'Sodium-Ion Battery Builder'* chatbot (Figure 5) that can be queried to find relevant mitigation strategies for a given macro- or micro-challenge. The chatbot can also handle queries for retrieving linked micro-challenges for a given macro-challenge. Additionally, it can be used to supply users with Digital Object Identifiers (DOI) linked to the scientific information it retrieves, enhancing reliability and reducing the risk of providing inaccurate information. Our database adopts a selective approach, concentrating on segments of the paper that address specific challenges and their respective mitigation strategies for SIBs that would not exceed the context window limitations of generative language models. Constructing specialized LLMs by incorporating entire research papers is impractical given the extensive quantity and size of these documents. Our targeted filtration enables efficient querying for this Retrieval Augmented Generation chatbot.

4 Limitations and Future Outlook

SIBs are a promising energy storage option due to the use of abundant and affordable element-containing precursors. NLP-extracted databases of synthesis and mitigation strategies have the potential to accelerate future research and industrialization, bringing the field closer to realizing the full potential of commercial SIBs. However, our methodology poses certain limitations. Firstly,

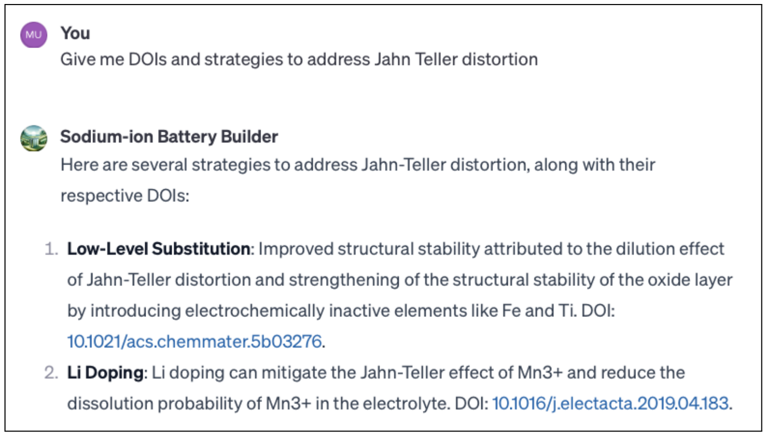

Figure 5: **'Sodium-ion Battery Builder' GPT** Snapshot of the chatbot to interact with the extracted database using OpenAI custom GPTs. The chatbot can be queries to understand underlying mechanistic causes of challenges encountered in battery development as well as strategies to address them from reliable sources.

NLP-extracted databases depend heavily on the quality and representativeness of the source data. There's a risk of bias as the literature used might disproportionately represent certain types of research over others. Secondly, the field of battery technology is rapidly evolving. Strategies identified as optimal today may become obsolete tomorrow as the field continues to develop a better understanding. Finally, transitioning from identifying Challenge-Mitigation patterns to selecting the optimal strategy remains a complex task necessitating human expertise. While NLP can identify patterns and suggest strategies, it lacks the intuition and expertise of human researchers. Using a human-in-loop approach, our NLP tool can be used to select strategies that can be economically viable at scale by integrating techno-economic cost-modeling approaches. Similarly, the tool can also be used to integrate with the assessment of other metrics like life cycle analyses for comparing mitigation strategies and synthesis pathways.

Furthermore, future applications may involve transferring the developed classifiers to the domain of LIB literature. Extracting related materials modification strategies from LIB literature, the established database could be augmented by LIB related mitigation strategies. This can potentially enable cross-domain knowledge transfer to SIB development by leveraging suitable mitigation strategies from LIBs.

5 Data Availability

The extracted database and classifiers are available at *github.com/olivettigroup/NLP4SIB*. Sodium Ion Battery Builder GPT built on OpenAI's ChatGPT platform as a custom GPT is available here: *chat.openai.com/g/g-2gOTffBeL-sodium-ion-battery-builder*.

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