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Semi-automatic staging area for high-quality structured data extraction from scientific literature

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ABSTRACT

We propose a semi-automatic staging area for efficiently building an accurate database of experimental physical properties of superconductors from literature, called SuperCon², to enrich the existing manually-built superconductor database SuperCon. Here we report our curation interface (SuperCon² Interface) and a workflow managing the state transitions of each examined record, to validate the dataset of superconductors from PDF documents collected using Grobid-superconductors in a previous work. This curation workflow allows both automatic and manual operations, the former contains ‘anomaly detection’ that scans new data identifying outliers, and a ‘training data collector’ mechanism that collects training data examples based on manual corrections. Such training data collection policy is effective in improving the machine-learning models with a reduced number of examples. For manual operations, the interface (SuperCon² interface) is developed to increase efficiency during manual correction by providing a smart interface and an enhanced PDF document viewer. We show that our interface significantly improves the curation quality by boosting precision and recall as compared with the traditional ‘manual correction’. Our semi-automatic approach would provide a solution for achieving a reliable database with text-data mining of scientific documents.

ARTICLE HISTORY

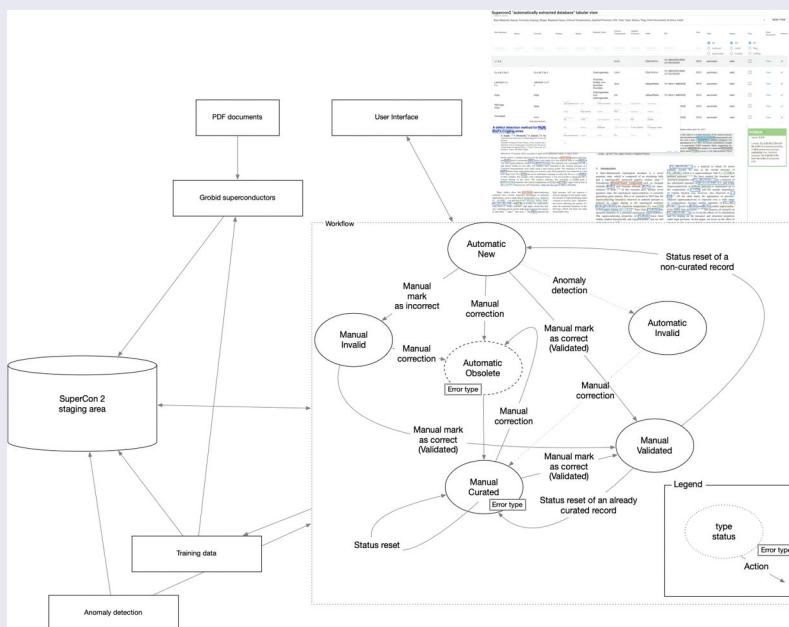
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KEY WORDS

Materials informatics;
superconductors; machine
learning; database; TDM



IMPACT STATEMENT

This work makes a contribution to the realms of materials informatics and superconductors research, achieved through the evolution and update of SuperCon. We provide results from experiments that support the utilisation of computational analysis and machine learning for collecting experimental data from scientific articles.

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1. Introduction

The emergence of new methodologies using machine learning for materials exploration has given rise to a growing research area called materials informatics (MI) [1,2]. This field leverages the knowledge of the materials data accumulated in the past to efficiently screen candidates of the materials with desired properties. As a matter of course, such an approach requires a larger amount of material-related data for training models. Researchers have been developing large aggregated databases of physical properties generated by first-principles calculations based on Density Functional Theory (DFT), such as Materials Project [3], JARVIS (Joint Automated Repository for Various Integrated Simulations) [4], NOMAD (Novel Materials Discovery) [5], that played a role of a strong driving force for the development of materials informatics. Using DFT data for machine learning (ML) in materials science has become popular since, in principle, it allows researchers to simulate and obtain various types of physical properties of the target materials only by knowing the crystal structures of the subjects. Those DFT codes are designed to reproduce/simulate the physical properties that should be observed by experiments in reality. Nonetheless, caution must be exercised while utilising these computed figures for constructing ML models aimed at steering experiments. This caution arises due to the potential lack of validity in their predictions when dealing with specific simplifications of the interactions between atoms and electrons in solids, such as electron-electron Coulomb correlation, spin-orbit coupling, and similar factors.

On the contrary, accumulated datasets of experimental data from scientific publications are still scarce, despite abundant publication availability, and exponential growth in materials science [6]. Currently, only a few limited resources exist, such as the Pauling File [7] and SuperCon [8], necessitating reliance on manual extraction methods. This scarcity can be attributed to inadequate infrastructure and a shortage of expertise in computer science within the materials science field.

The SuperCon database was built manually from 1987 [8] by the National Institute for Materials Science (NIMS) in Japan and it is considered a reliable source of experimental data on superconductors [9–12]. However, the updates of SuperCon have become increasingly challenging due to the high publication rate. In response to the need for a more efficient approach to sustain productivity, we embarked on the development of an automated system for extracting material and property information from the text contained in relevant scientific publications. This automated process enabled the rapid creation of ‘SuperCon² Database’, a comprehensive database of superconductors containing around 40,000 entries,

within an operational duration of just a few days [1]. Matching the level of quality seen in SuperCon while simultaneously automating the extraction of organised data can be achieved with a properly designed curation process. We use the term *curation* to describe the overall process of reviewing and validating database records, while *correction* refers to the specific action of altering the values of one or more properties within an individual record. At the moment of writing this article, we are not aware of any other curation tool focusing on structured databases of extracted information. There are several tools for data annotation, such as Inception [13], and Doccano [14] which concentrate on text labelling and classification.

In this work, we designed and developed a workflow with a user interface, ‘SuperCon² Interface’, crafted to produce structured data of superior quality and efficiency to the one obtained by the ‘traditional’ manual approach consisting of reading documents and noting records, usually on an Excel file. We developed this framework around the specific use case of SuperCon, however, our goal is to be adapted to alternative data frameworks.

Our contributions can be summarised as follows:

- We developed a workflow and a user interface that allow the curation of a machine-collected database. We demonstrate that using it for data correction resulted in higher quality than the ‘traditional’ (manual) approach.
- We devise an anomaly detection process for incoming data lower rejection rate (false positive rate) from domain experts.
- We propose a mechanism that selects training data based on corrected records, and we demonstrate that such selections are rapidly improving the ML models.

The subsequent sections, [Section 2](#) describes the curation workflow and [Section 3](#) the user interface on top of it. Finally, we discuss our evaluation experiments and results in [Section 4](#).

2. Curation workflow

The curation of the SuperCon² Database acts as a workflow where user actions result in database records state transitions ([Figure 1](#)). Allowed manual actions include a) *mark as valid* (validation) when a record is considered correct or corrected by someone else. When a record is not valid, users can: b) *mark as invalid* when considered ‘potentially’ invalid (or the curator is not confident), c) perform *manual correction* to update it according to the information from the original PDF document, and d) *remove* the record when it was not supposed to be extracted.

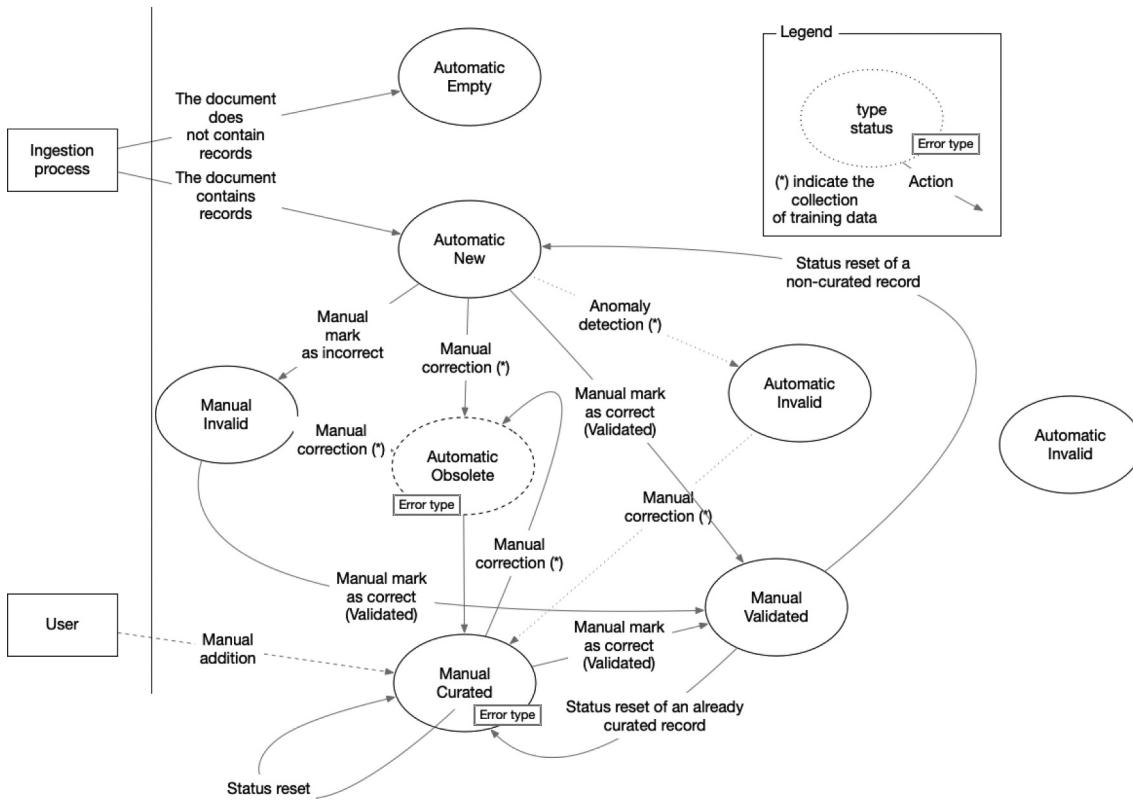


Figure 1. Schema of the curation workflow. Each node has two properties: type and status (Section 2.1.1). Each edge indicates one action. The workflow starts on the left side of the figure. The new records begin with ‘automatic, new’. Changes of state are triggered by automatic (Section 2.2) or manual operations (update, mark as valid, etc. Section 3.1) and results in changes of the properties in the node. Each combination of property values identifies each state. ‘(*)’ indicates a transition for which the training data are collected (Section 2.3).

Besides manual operations from users, this workflow supports also automatic actions: ‘anomaly detection’ for pre-screening records (Section 2.2) and the ‘training data collector’ for accumulating training data for improving ML models (Section 2.3).

Although only the most recent version of a record can be viewed on this system, the correction history is recorded (Section 3.3).

2.1. Workflow control

The workflow state is determined by the ‘curation status’ (Section 2.1.1), the user action, and the error type (Section 2.1.2).

2.1.1. Curation status

The curation status (Figure 1) is defined by *type* of action, manual or automatic, and *status*, which can assume the following values:

- **new:** default status when a new record is created.
- **curated:** the record has been amended manually.
- **validated:** the record was manually marked as valid.
- **invalid:** the record is wrong or inappropriate for the situation (e.g. T_m or T_{curie} extracted as superconducting critical temperature).

- **obsolete:** the record has been updated and the updated values are stored in a new record (internal status¹).
- **removed:** the record has been removed by a curator (internal status).

2.1.2. Error types

We first introduced *error type* in [1] and extended their scope in this work to consider data curation and anomaly detection.

Users are required to select one *Error Type* at every record update or removal. This information is stored in the ‘original’ record and can be different at every record modification. The error type values can be summarised as follows:

- **From table:** the entities Material → T_c → Pressure are identified in a table. At the moment, table extraction is not performed
- **Extraction:** The material, temperature, and pressure are not extracted (no box) or extracted incorrectly.
- **Linking:** The material is incorrectly linked to the T_c given that the entities are correctly recognised.
- **T_c classification:** The temperature is not correctly classified as ‘superconductors critical temperature’ (e.g. Curie temperature, Magnetic temperature...).

- **Composition resolution:** The exact composition cannot be resolved (e.g. the stoichiometric values cannot be resolved).
- **Value resolution:** The extracted formula contains variables that cannot be resolved, even after having read the paper. This includes when data is from tables
- **Anomaly detection:** The data has been modified by anomaly detection, which facilitates their retrieval from the interface.
- **Curation amends:** The curator is updating the data which does not present issues due to the automatic system.

2.2. Anomaly detection

Anomaly detection is the process of identifying unusual events or patterns in data. In our context, this means identifying data that are greatly different from the expected values. This post-process was introduced in a limited scope to draw attention to certain cases during the curation.

The anomaly detection uses a rule-based approach and marks any record that matches the following conditions

- the extracted T_c is greater than room temperature (273 K), negative, or contains invalid characters and cannot be parsed (e.g. '41')
- the chemical formula cannot be processed by an ensemble composition parser that combines Pymatgen [15], and text2chem [16]
- the extracted applied pressure cannot be parsed or falls outside the range 0–250 GPa.

Records identified as anomalies have *status* 'invalid' and *error type* 'anomaly detection' for easy identification. Since this process may find false positives, its output requires validation from curators. For example, in certain contexts, T_c values above room temperature or applied pressure up to 500 GPa may be valid in researchers' hypotheses, calculations, or simulated predictions.

We ran the anomaly detection on the full SuperCon² Database (40324 records [1]). The anomaly detection identified 1506 records with invalid T_c , 5021 records with an incomplete chemical formula, 304 records with invalid applied pressure, and 1440 materials linked to multiple T_c values. Further analysis and cross-references with contrasting information may be added in future.

2.3. Automatic training data collector

The curation process is a valuable endeavour demanding significant knowledge and human effort. To maximise the use of this time for collecting as much information as possible. We integrated an automatic procedure in the curation process that, for every

correction, accumulates the related data examples that can be used to improve the underlying ML models.

2.3.1. Training data collection

In the event of a correction (update, removal) in a database record, this process retrieves the corresponding raw data: the text passage, the recognised entities (spans), and the layout tokens information. This information is sufficient to be exported as training examples, which can be examined and corrected, and feedback to the ML model.

2.3.2. Training data management

We designed a specific page of the interface (Section 3) to manage the collected data (Figure 2) in which each row corresponds to a training example composed by the decorated text showing the identified entities, the document identifier, and the status. The users can examine the data, delete it, send it to the annotation tool to be corrected, and then export them. We integrated our interface with Label-studio [17] for the correction of the collected training examples. Label-studio is an open-source, python-based, and modern interface supporting many different TDM tasks (NER, topic modelling, image recognition, etc.).

3. Curation interface

The workflow is operated through the user interface, which offers several key features to facilitate the data curation process (Figure 1). It provides a comprehensive view of materials and their related properties as a table which includes search, filtering, and sorting functionality (Figure 3). The detailed schema, including examples, is reported in our previous work [1].

During the curation process, it is often necessary to switch back and forth between the database record and the related context in the paper (the related paragraph or sentence). Our interface provides a viewer for individual documents, which visualises in the same window a table with the extracted records and the original PDF document decorated with annotations that identify the extracted materials and properties (Figure 4).

3.1. Manual curation approach

In this section, we discuss our strategy concerning manual curation, which is still indispensable for developing high-quality structures.

We selected curators from domain experts in the field, to certify sufficient data quality. Nevertheless, as confirmed from our experiment in Section 4.3, the experience of each individual may have an impact on the final result. We followed two principles to guarantee robustness in the curation process. First, we built solid curation documentation as a form of example-driven guidelines with an iterative approach we first introduced in [18]. Then, we used a double-round validation approach, in

SuperCon² | Training data viewer

Select Columns
Text, Status, Document, Actions

Settings for enabling authentication to label-studio
SEND ALL TOKEN
Indicate whether the training data has been sent to label-studio

Status	Document	Actions
in_progress	f2fe747414	▶ <input type="checkbox"/>
in_progress	68bae90b9a	▶ <input type="checkbox"/>
in_progress	f2fe747414	▶ <input type="checkbox"/>
in_progress	f2fe747414	▶ <input type="checkbox"/>
in_progress	00eafe0a38	▶ <input type="checkbox"/>
in_progress	9273cb60e2	▶ <input type="checkbox"/>
in_progress	48ba234393	▶ <input type="checkbox"/>
in_progress	d143899d50	▶ <input type="checkbox"/>
in_progress	0032e3090a	▶ <input type="checkbox"/>
in_progress	00eafe0a38	▶ <input type="checkbox"/>
in_progress	48ba234393	▶ <input type="checkbox"/>
in_progress	a78145fbef	▶ <input type="checkbox"/>
in_progress	9ad40af6e2	▶ <input type="checkbox"/>
new	9ad40af6e2	▶ <input type="checkbox"/>

Text
An example is the indium (In)-doped many-valley semiconductor tin-telluride (SnTe) where a maximum superconducting transition temperature of ~4.4 K is reported for $x \sim 0.5$ in the series $\text{Sn}_{1-x}\text{In}_x\text{Te}$ [3, 6, 7].
For instance, partial substitution of Te for Se (chemical pressure effect) leads to an increase in T_c up to 11.5 K with 0.3×0.7 for $\text{FeSe}_{1-x}\text{Te}_x$ compounds, 3.4 while application of external pressure of 8.9 GPa (Refs.).
Superconductivity appears in Bi_2Se_3 at ~13.5 GPa at a transition temperature of 0.5 K which gradually increases to a maximum of 7 K on increasing pressure up to 30 GPa.
This is schematically shown in figure 2. From figure 2, the values of T_c onset, T_c offset and T_c zero c for single-crystal Sn 0.5 In 0.5 Te are found to be 4.4 K, 4.1 K and 3.6 K respectively.
We carried out the resistivity measurement using the fresh as-cleaned surface of the $\text{K}_{0.8}\text{Fe}_{2}\text{Se}_2$ crystal and observed a high T_c onset of 33 K.
Very recently, an isostructural $\text{LaO}_{1-x}\text{FeO}_x$ compound has been reported to exhibit enhanced-superconductivity with T_c of 3.5 K [17, 18] compared to the low- T_c phase in $\text{LaO}_{1-x}\text{Fe}_x\text{BiS}_2$ [5, 15].
It has the value of 27 K and is higher than T_c of single crystals (23 K and 22 K) 22.3 and thin films (24.5 K). 24 Recent results show that The $(\text{Ca},\text{Ce})_{12}$ compounds with RE = La, Pr, Nd, Sm, Eu and Gd exhibited superconductivity, while the $(\text{Ca},\text{Ce})_{12}$ compound did not show superconductivity, even at temperature as low as 2 K. Kudo et al reported that the double-doping of $(\text{Ca},\text{RE})_{12}$ with SB increased the T_c to 47, 43, 43, and 43 K for RE = La, Ce, Pr, and Nd, respectively [13]. Notice that, high-pressure metallic phases of the elements and compounds of VI-VII groups are often super-conducting (e.g., in elemental sulfur T_c of 10–17 K at 90–160 GPa), 57,58 and hence, one could also anticipate this effect in $\text{Sn}_{2}\text{P}_{2}\text{S}_6$.
An outstanding example is the pressure effect of FeSe , the T_c shows a huge increase from 13 to 37 K under 4.6 GPa 10-13 and the large enhancement of T_c in FeSe is strongly related to the change in the anion height.
Our research suggests that the HIP at 1 GPa leads to high T_c (27 K) and high B_c2 in $\text{Ba}(\text{FeCo})_2\text{As}_2$ material with critical temperatures of 27 K and 21.5 K at upper critical flux density (B_c2) of 14 T.
The analysis indicates that annealing at 1 GPa leads to the $\text{Ba}(\text{FeCo})_2\text{As}_2$ material with critical temperatures of 27 K and 21.5 K at upper critical flux density (B_c2) of 14 T.
 $\text{Bi}_2\text{NiTiO}_6$ compound which shows both magnetic (T_M = 58 K) and ferroelectric properties (T_C = 513 K) was synthesized under high pressure of 5 GPa and temperature of 1273 K.
It was generally considered that H_2S may dissociate under high pressure, and it is H_3S that records high-temperature superconductivity with the T_c of 203 K, 23-25) The various stoichiometry and structures of hydrogen sulphide have been extensively studied, 26-28 and the decomposition paths of H_2S were predicted as $\text{H}_2\text{S} \rightarrow (28 \text{ GPa}) \text{H}_3\text{S} + \text{H}_3\text{S}_2 \rightarrow (42 \text{ GPa}) \text{H}_3\text{S} + \text{H}_5\text{S}_2 \rightarrow (112 \text{ GPa}) \text{H}_3\text{S} + \text{H}_5\text{S}_2 \rightarrow \text{H}_3\text{S} + \text{S}$ 29) However, there is still controversy about the stoichiometry and structures of hydrogen sulphide which account for high- T_c , e.g., the experimental XRD at 180 GPa showed that the diffraction peak intensity of S is much smaller than expected. 30)
The superconducting transition temperature of the $\text{C}_2\text{m}-\text{H}_2\text{S}$ structure was predicted to be 53–74 K at 150 GPa.

Figure 2. Screenshot of the training data management page in the SuperCon² interface. Each row contains one potential training data example. Each example is composed of a sentence and its extracted entities (highlighted in colour) with potential annotation mistakes that need to be corrected using an external tool: we used label-studio [17]. The column ‘status’ indicate whether the example has been sent or not to the external tool.

SuperCon² | Database

Select Columns
Formula, Shape, Material Class, Critical Temperature, Applied Pressure, Document, DOI, Sentence, Status, Actions

Formula	Shape	Material Class	Critical Temperature	Applied Pressure	Document  1	DOI	Sentence	Status	Actions
keyword	keyword	keyword	keyword	keyword	keyword	keyword	keyword	all	
CeAg ₂ Si ₂	crystals	Alloys	1.25 K	16 GPa	03867972c6 	10.1016/j.physb.2017.09.120	We scanned the pressure-temper ...	new	
Sm _{1.11} Ba _{1.89} Cu ₃ O _{6.95}	crystals	Oxides, Cuprates	94.5 K	1 bar	03e8c2fa2b 	10.1016/j.tca.2004.04.026	Their T_c value is 94.5 K. Sm ...	new	
CeAu ₂ Si ₂	single crystals	Alloys	2.5 K	up to 27.4 GPa	04df799f8e 	10.1103/physrevx.4.031055	In this paper, we report on pr ...	new	
NdFeAsO _{0.82} F _{0.18}	single crystals	Iron-prictides, Oxides, Prictides, Fluorides	47 K	ambient pressures	12bee124b6 	10.1088/0953-2048/25/11/113001	Jia et al. have first grown si ...	new	
Sr ₄ V ₂ O ₆ Fe ₂ As ₂	polycrystalline	Iron-prictides, Prictides, Oxides	from 15 to 22 K	1.2 GPa	1a6cb866c4 	10.1038/srep08213	Our results show that pressure ...	new	
KOs ₂ O ₆	single crystal	Oxides	from 6.5 to 3.3 K	3.	1c854024a7 	10.1143/jpsj.80.104708	Recently, Ogusu et al. have ca ...	new	
RbOs ₂ O ₆	single crystal	Oxides	9.3 K	3 GPa	1c854024a7 	10.1143/jpsj.80.104708	In contrast, the pressure dep ...	new	
2H-NbSe ₂	single crystal	Alloys	6.0 K	0	1e543679c5 	10.1007/bf02704945	In the panel (d), the χ' ω da ...	invalid	
CeRu ₂	crystal	Alloys	6.3 K	0	1e543679c5 	10.1007/bf02704945	In the panel (d), the χ' ω da ...	new	

Figure 3. Screenshot of SuperCon² interface showing the database. Each row corresponds to one material- T_c pair. On top, there are searches by attribute, sorting and other filtering operations. On the right there are curation controls (mark as valid, update, etc.). Records are grouped by document with alternating light yellow and white.

which the data was initially corrected by one person, and validated in a second round, by a different individual.

3.2. Curation guidelines

The guidelines consist mainly of two parts: the general principles and the correction rules with examples of solutions. The guidelines are designed to provide general information applied to corrections and very basic explanations containing illustrations for a faster understanding (e.g. the meaning of the colours of the annotations).

Differently from our previous work [18], these guidelines are divided into examples for different scenarios based on the error types mentioned in Section 2.1.2. Each example described the initial record, its context, the expected corrected record and a brief explanation, as illustrated in Figure 5.

3.3. Curation and processing logs

The Supercon² interface gives access to information regarding the ingestion (processing log) and the

Formula	Critical Temperature	Applied Pressure	Sentence	Status	Actions
MgB ₂	39 K	0 GPa	In fact, MgB ₂ was considered ...	curated	

X **T_c** and **T_c**, respectively.³³ According to the obtained results, **H₂S** dissociates in phase V; thus, Drozov and coworkers performed compression at a low temperature of 200 K to avoid this region and achieve a "high-*T_c" phase".¹¹ Electrical resistance starts to decrease at around 50 GPa³⁴ and superconductivity is observed above 100 GPa³⁵ and **T_c** becomes 150 K at around 200 GPa³⁶. The high-*T_c" phase including the **T_c** of 200 K is obtained by annealing at around 150 GPa³⁷ at room temperature. From the electrical resistance measurements in its isotope deuterium sulfide (D₂S), Drozov and coworkers argued that the high-*T_c" phase has a conventional superconductivity because of its isotope effect on superconductivity. The superconductivity was confirmed not only by electrical resistance measurement but also by the Meissner effect.¹¹***

The predicted **T_c** of 80 K for **H₂S** is consistent with the experimentally observed superconductivity in the low-*T_c" phase.¹¹ However, the **T_c** of 200 K does not follow the predicted value. Thus, it was suggested that **H₂S** is decomposed to sulfur hydride with a higher hydronium content*

Bardeen-Cooper-Schrieffer (BCS) theory³⁸ are considered "conventional" (● in Fig. 1). On the basis of this theory, Ascroft predicted that metallic hydrogen will become a high-*T_c" superconductor.³⁹ For metallization, however, an extremely high pressure will be required (above 400 GPa⁴⁰ as predicted by recent theoretical prediction³⁰). On the other hand, the maximum **T_c** was predicted to be 40 K on the basis of the BCS theory. In fact, MgB₂ was considered as a conventional superconductor with the highest **T_c** of 39 K.⁴¹ The predicted metallization pressure above 400 GPa has not yet been achieved. In 2004, Ascroft predicted that hydrides will change to metallic and superconducting at much lower pressures than the case of pure hydrogen.⁴¹ On the basis of this prediction, some superconductors in hydrides have been examined theoretically, but only **T_c** = 17 K silane (SiH₄) has been observed experimentally thus far.³²*

It is considered that the two-dimensional layered structure of unconventional superconductors contributes to a high **T_c**. The highest **T_c** values of 134 K under ambient pressure and 173 K at a high pressure were found in Mg_{1-x}Ni_x³³ in

Figure 4. PDF document viewer showing an annotated document. The table on top is linked through the annotated entities. The user can navigate from the record to the exact point in the PDF, with a pointer (the red bulb light) identifying the context of the entities being examined.

• Sample input data															
Raw Material	Name	Formula	Doping	Variables	Fabrication	Critical Temperature	Applied Pressure	Measurement Method	Document ↑	DOI	Flag	Actions			
Cu _{0.25} Bi ₂ (Te _{0.01} Se _{0.99}) ₃	Cu _{0.25} Bi ₂ (Te _{0.01} Se _{0.99}) ₃					3.2 K	1 GPa	resistivity	11d82d01fc	10.7567/JJAP.56.05FB04	<input checked="" type="checkbox"/>				

• Context												
First, we discuss the drop in resistivity at ambient pressure and its disappearance by compression. Assuming that this drop and diamagnetism are due to superconductivity in Cu _{0.25} Bi ₂ (Te _{0.01} Se _{0.99}) ₃ we can consider that the superconducting transition at T_c = 3.2 K vanishes at P = 1 GPa.												

• Motivation												
The system failed to link the correct items (formula-Tc-pressure) (here, at P=1 GPa, superconductivity vanishes, and Tc = 3.2K is a value for ambient pressure)												

• Action												
Edit -> Set "pressure" to "0 GPa"												

• Expected output															
Raw Material	Name	Formula	Doping	Variables	Fabrication	Critical Temperature	Applied Pressure	Measurement Method	Document ↑	DOI	Flag	Actions			
Cu _{0.25} Bi ₂ (Te _{0.01} Se _{0.99}) ₃	Cu _{0.25} Bi ₂ (Te _{0.01} Se _{0.99}) ₃					3.2 K	0 GPa	resistivity	11d82d01fc	10.7567/JJAP.56.05FB04	<input checked="" type="checkbox"/>				

Figure 5. Sample curation sheet from the curation guidelines. The sheet is composed of the following information: (a) Sample input data: a screenshot of the record from the 'SuperCon² interface', (b) Context represented by the related part of the annotated document referring to the record in exams. (c) The Motivation, describing the issue, (d) The Action to be taken, and the expected output.

curation process (curation log). The processing log is filled up when the new data is ingested, it was built to have minimal functions able to explain why certain documents haven't been processed (Figure 6 top). For example, sometimes documents fail because they don't contain any text (image PDF documents) or they are too big (more than 100 pages).

The curation log provides a view of what, when and how a record has been corrected (Figure 6 bottom).

4. Results and evaluation

In this section, we illustrate the experiments we have run to evaluate our work. The evaluation is composed of three sets of results. The anomaly detection rejection rate (Section 4.1) indicates how many anomalies were rejected by curators after validation. Then, we demonstrate that the training data automatically

selected contributed to improving the ML model with a small set of examples (Section 4.2) Finally, we evaluated the quality of the data extraction using the interface (and the semi-automatic TDM process) against the classical method of reading the PDF articles and noting the experimental information in an Excel file. In Section 4.3 we find out that using the interface improves the quality of the curated data by reducing missing experimental data.

4.1. Anomaly detection rejection rate

We evaluated the anomaly detection by observing the 'rejection rate' which consists of the number of detected anomalies that were rejected by human validation. Running the anomaly detection on a database subset with 667 records, it found 17 anomalies in T_c, 1 anomaly in applied pressure, and 16 anomalies in the chemical

SuperCon ² Processing log					Service	Path	Document ↑ ②	Timestamp ↓ ①	Status
Message					extraction	keyword	keyword	keyword	all
Exception				x					
org.grobid.core.exceptions.GrobidException [GENERAL] Cannot process input file. org.grobid.core.exceptions.GrobidException: [PDFALTO_CONVERSION_FAILURE] PDF to XML conversion failed on pdf file /opt/grobid/grobid-home/tmp /origin894488326384040027.pdf					extraction	./corrected_documents_sakai /f58a9d98f1.pdf	6c958ff1f18	1/14/22, 2:50 PM	500
org.grobid.core.exceptions.GrobidException [GENERAL] Cannot process input file. org.grobid.core.exceptions.GrobidException: [PDFALTO_CONVERSION_FAILURE] PDF to XML conversion failed on pdf file /opt/grobid/grobid-home/tmp /origin781394020416367.pdf					extraction	./corrected_documents_sakai /f2fe747414.pdf	975d147fc9	1/14/22, 2:50 PM	500
org.grobid.core.exceptions.GrobidException [GENERAL] Cannot process input file. org.grobid.core.exceptions.GrobidException: [PDFALTO_CONVERSION_FAILURE] PDF to XML conversion failed on pdf file /opt/grobid/grobid-home/tmp /origin325254549490230814.pdf					extraction	./corrected_documents_sakai /f2132da875.pdf	b7cf11c03	1/14/22, 2:50 PM	500

SuperCon ² Correction log					Latest error type	Status
Record id	Update count	Document	Timestamp ↓ ①	DOI		
keyword	keyw	keyword	keyword	keyword	All	all
63f5f6769d2b56b182455e36e	1	14fcc539b1	2/22/23, 9:52 AM	10.1088/1361-6668/aac246	composition_resolution	curated
633fd2018fa3814924f69aef	0	14fcc539b1	2/9/23, 10:21 AM	10.1088/1361-6668/aac246	tc_classification	removed
633fd2018fa3814924f69af0	0	14fcc539b1	2/9/23, 10:21 AM	10.1088/1361-6668/aac246	tc_classification	removed
633fd2018fa3814924f69af8	0	14fcc539b1	2/9/23, 10:15 AM	10.1088/1361-6668/aac246	tc_classification	removed
633fd2018fa3814924f69af3	0	14fcc539b1	2/9/23, 10:08 AM	10.1088/1361-6668/aac246	tc_classification	removed
633fd1ff8fa3814924f69ab6	0	139f820e67	2/2/23, 10:37 AM	10.1063/1.5053650	extraction	removed

Figure 6. Top: *Processing log*, showing the output of each ingestion operation and the outcome with the detailed error that may have occurred. Bottom: *Correction log*, indicating each record, the number of updates, and the date/time of the last updates. By clicking on the ‘record id’, is possible to visualise the latest record values.

formulas. Curators examined each reported record and rejected 4 (23%) anomalies in T_c , 6 anomalies (37%) in chemical formulas and 0 anomalies in applied pressure. This indicates an appropriate low rate of false positives although a study with a larger dataset might be necessary.

4.2. Training data generation

We selected around 400 records in the Supercon² Database that were marked as invalid by the anomaly detection process and we corrected them following the curation guidelines (Section 3.2). Then, we examined the corresponding training data corrected by the interface (Section 2.3) and obtained a set of 352 training data examples for our ML models. We call the obtained dataset *curation* to be distinguished from the original SuperMat dataset which is referred to as *base*.

We prepared our experiment using SciBERT [19] that we fine-tuned for our downstream task as in [1]. We trained five models that we evaluated using a fixed holdout dataset from SuperMat averaging the results to smooth out the fluctuations. We use the DeLFT (Deep Learning For Text) [20] library for training, evaluating, and managing the models for prediction. A model can be trained with two different strategies:

- (1) ‘from scratch’: when the model is initialised randomly. We denote this strategy with an (s).
- (2) ‘incremental’: when the initial model weights are taken from an already existing model. We denote this strategy with an (i).

The latter can be seen as a way to ‘continue’ the training from a specific checkpoint. We thus define three different training protocols:

- (1) **base(s)**: using the *base* dataset and training from scratch (s).
- (2) **(base+curation)(s)**: using both the *base* and *curation* datasets and training from scratch (s).
- (3) **base(s)+(base+curation)(i)**: Using the *base* dataset to train from scratch (s), and then continuing the training with the *curation* dataset (i).

We merge ‘curation’ with the base dataset because the curation dataset is very small compared to ‘base’, and we want to avoid catastrophic forgetting [21] or overfitting.

The trained models are then tested using a fixed holdout dataset that we designed in our previous work [1] and the evaluation scores are shown in Table 1.

This experiment demonstrates that with only 352 examples (2% of the SuperMat dataset) comprising 1846 additional entities (11% of the entities from the SuperMat dataset) (Table 2), we obtain an improvement of F1-score from 76.67%² to values between

Table 1. F1-score from the evaluation of the fine-tuned SciBERT models. The training is performed with three different approaches. The *base* dataset is the original dataset described in [18], and the *curation* dataset is automatically collected based on the database corrections by the interface and manually corrected. s indicate ‘training from scratch’, while i indicate ‘incremental training’. The evaluation is performed using the same holdout dataset from SuperMat [18]. The results are averaged over five runs or train and evaluation.

	(base+curation) base(s)	(base+curation) (s)	base(s)+(base+curation)(i)
Nb total examples	16902	17254	16902(s), 17254 (i)
<class>	70.41	73.02	71.86
<material>	79.37	80.09	80.37
<me_method>	66.72	66.57	66.95
<pressure>	46.43	48.42	47.23
<tc>	80.13	80.92	80.34
<tcValue>	78.29	78.41	79.73
All (micro avg.)	76.67	77.44	77.48
Δ avg. w/baseline	-	+0.77	+0.81

Table 2. Data support, the number of entities for each label in each of the datasets used for evaluating the ML models. The *base* dataset is the original dataset described in [18], and the *curation* dataset is automatically collected based on the database corrections by the interface and manually corrected.

	base	base+curation	Δ
<class>	1646	1732	86
<material>	6943	7580	637
<me_method>	1883	1934	51
<pressure>	274	361	87
<tc>	3741	4269	528
<tcValue>	1099	1556	457
Total	15586	17432	1846

77.44% (+0.77) and 77.48% (+0.81) for (base+curation)(s) and base(s)+(base+curation)(i), respectively.

This experiment gives interesting insight relative to the positive impact on the way we select the training data. However, there are some limitations: the *curation* dataset is small compared to the *base* dataset. This issue could be verified by correcting all the available training data, repeating this experiment, and studying the interpolation between the size of the two datasets and the obtained evaluation scores. A second limitation is that the hyperparameters we chose for our model, in particular, the learning rate and batch size could be still better tuned to obtain better results with the second and third training protocols.

4.3. Data quality

We conducted an experiment to evaluate the effectiveness and accuracy of data curation using two methods: a) the user interface (*interface*), and b) the ‘traditional’ manual approach consisting of reading PDF documents and populating an Excel file (*PDF documents*).

We selected a dataset of 15 papers, which we assigned to three curators – a senior researcher (SD), a PhD student (PS), and a master’s student (MS). Each curator received 10 papers: half to be corrected with the *interface* and half with the *PDF Document* method. Overall, each pair of curators had five papers in common which they had to process using opposite methods. For instance, if curator A receives paper 1 to be corrected with the *interface*, curator B, who receives the same paper 1, will correct it with the *PDF document* method. After curation, a fourth individual manually reviewed the curated content. The raw data is available in Tables A1 and A2.

We evaluated the curation considering a double perspective: time and correctness. Time was calculated as the accumulated minutes required using each method. Correctness was assessed using standard measures such as precision, recall, and the F1-score. Precision measures the accuracy of the extracted information, while recall assesses the ability to capture all expected information. F1-Score is a harmonic means of precision and recall.

4.3.1. Discussion

Overall, both methods required the same accumulated time: 185 minutes using the *interface* and 184 minutes using the *PDF Document* method. When the experiment was carried out, not all the curators were familiar with the *interface* method. Although they had access to the user documentation, they had to get acquainted with the user interface, thus the accumulated 185 minutes included such activities.

We examined the quality of the extracted data and we observed an improvement of + 5.55% in precision and a substantial + 46.69% in recall when using the *interface* as compared with the *PDF Document* method (Table 3). The F1-score improved by 39.35%.

The disparity in experience significantly influenced the accuracy of curation, particularly in terms of high-level skills. Senior researchers consistently achieved an average F1-Score approximately 13% higher than other curators (see Table 4). Furthermore, we observed a modest improvement between master’s students and PhD students. These findings indicate also that for large-scale projects, employing master students instead of PhD students may be a more cost-effective choice. Thus, using only a few senior researchers for the second round of validation (Section 3.1).

Finally, the collected data suggest that all three curators had overall more corrected results by using the *interface* as illustrated in Table 5.

The results of this experiment confirmed that our curation interface and workflow significantly improved the quality of the extracted data, with an astonishing improvement in recall, thus preventing curators from overlooking important information.

5. Code availability

This work is available at <https://github.com/lfoppiano/supercon2>. The repository contains the code of the SuperCon² interface, the curation workflow, and the

Table 3. Evaluation scores (P: precision, R: recall, F1: F1-score) between the curation using the SuperCon² interface (*Interface*) and the traditional method of reading the PDF document (*PDF document*).

Method	P (%)	R (%)	F1%	# docs
PDF document	87.83	45.61	52.67	15
Interface	93.38	92.51	92.02	15

Table 4. Evaluation scores (P: precision, R: recall, F1: F1-score) aggregated by experience (MS: master student, PD: PhD student, SR: senior researcher). Each person corrected 10 documents.

Experience	P (%)	R (%)	F1%	# docs	# pages
MS	90.03	60.26	64.50	10	96
PD	83.33	65.69	69.45	10	100
SR	98.45	81.22	83.08	10	96

Table 5. Evaluation scores (P: precision, R: recall, F1: F1-score) listed by experience (MS: master student, PD: PhD student, SR: senior researcher), and method (PDF document, interface).

Experience	Method	P (%)	R (%)	F1%	# docs	# pages
MS	PDF Document	94.58	36.55	48.67	6	46
	Interface	83.19	95.83	88.25	4	50
PD	PDF Document	70.00	48.51	50.78	5	49
	Interface	96.67	82.86	88.11	5	51
SR	PDF Document	100.00	55.56	61.03	4	51
	Interface	97.42	98.33	97.78	6	45

ingestion processes for harvesting the SuperCon² Database of materials and properties. The guidelines are accessible at <https://supercon2.readthedocs.io>.

6. Conclusions

We built a semi-automatic staging area, called SuperCon², to validate efficiently new experimental records automatically collected from superconductor research articles (SuperCon² Database [1]) before they are ingested into the existing, manually-build database of superconductors, SuperCon [8]. The system provides a curation workflow and a user interface (SuperCon² Interface) tailored to efficiently support domain experts in data correction and validation with fast context switching and an enhanced PDF viewer. Under the hood, the workflow ran ‘anomaly detection’ to automatically identify outliers and a ‘training data collector’ based on human corrections, to efficiently accumulate training data to be feedback to the ML model.

Compared with the traditional manual approach of reading PDF documents and extracting information in an Excel file, SuperCon² significantly improves the curation quality by approximately 6% and + 47% for precision and recall, respectively. In future, this work can be expanded to support other materials science domains such as magnetic materials, spintronic and thermoelectric research and expanding the evaluation to a larger [22] dataset.

Notes

- ‘internal status’ indicates that their records should be hidden in the interface.
- In our previous work [1] we reported 77.03% F1-score. There is a slight decrease in absolute scores between DeLFT 0.2.8 and DeLFT 0.3.0. One cause may be the use of different hyperparameters in version 0.3.0 such as batch size and learning rate. However, the most probable cause could be the impact of using the Huggingface tokenizers library which is suffering from quality issues <https://github.com/kermitt2/delft/issues/150>.

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Disclosure statement

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Author contribution

LF wrote the manuscript and KT helped with the editing. LF and POS discussed the ML results and experiments. LF implemented the workflow as a standalone service, and TM wrote the front end of the user interface. LF designed the user interface experiment with KT, TT and WS as curators. KT led the materials-science work on the data with CS, TT and WS. KT, TA, YT and MI revised the paper. YT and MI supervised the work of the respective teams.

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Appendix A. Evaluation

Table A1. Timetable recording the time spent for each of the 15 articles. Each row indicates the time and the event (Start, Finish) from each of the curators: master student (MD), PhD student (PD), and senior researcher (SR). Duration is expressed in minutes.

Time	Event	Document ID	Curator	Duration (mins)
14:40	Start	02bf1b3db9	PS	0
14:49	Finish	02bf1b3db9	PS	9
14:53	Start	00b50fc0a8	PS	0
14:58	Finish	00b50fc0a8	PS	5
14:37	Start	0aa1b3161f	MS	0
14:50	Start	0454e07f64	SR	0
14:58	Finish	0454e07f64	SR	8
15:01	Start	02cbc58819	PS	0
15:06	Start	00c32076f4	SR	0
15:07	Finish	0aa1b3161f	MS	30
15:08	Finish	02cbc58819	PS	7
15:08	Start	044939701d	PS	0
15:12	Start	0021fd339f	MS	0
15:15	Finish	00c32076f4	SR	9
15:17	Finish	044939701d	PS	9
15:17	Start	08e1cb8f4f	PS	0
15:20	Start	0c7d3163ea	SR	0
15:31	Finish	08e1cb8f4f	PS	14
15:32	Finish	0021fd339f	MS	20
15:32	Start	039105663f	MS	0
15:37	Finish	0c7d3163ea	SR	17
15:53	Finish	039105663f	MS	21
15:55	Start	02c4f00127	MS	0
15:58	Start	0454e07f64	PS	0
16:02	Start	0da5febabb	SR	0
16:08	Finish	0454e07f64	PS	10
16:09	Finish	02c4f00127	MS	14
16:11	Finish	0da5febabb	SR	9
16:11	Start	0012333581	SR	0
16:12	Start	00c32076f4	PS	0
16:18	Start	021c413172	MS	0
16:22	Finish	00c32076f4	PS	10
16:23	Start	0c7d3163ea	PS	0
16:30	Finish	0012333581	SR	19
16:32	Finish	021c413172	MS	14
16:37	Start	02bf1b3db9	MS	0
16:38	Finish	0c7d3163ea	PS	15
17:32	Finish	0021fd339f	SR	12
17:34	Start	039105663f	SR	0
17:55	Finish	039105663f	SR	21
17:56	Start	02c4f00127	SR	0
18:00	Finish	02c4f00127	SR	4
18:00	Start	021c413172	SR	0
18:09	Finish	021c413172	SR	9

Table A2. Evaluation scores obtained for each document and method (I: interface, P: PDF) combination. TP: true positive, FP: false positive, FN: false negative. P: precision, R: recall, F1: F1-score.

Document ID	# pages	Method	# TP	# FP	# FN	P	R	F1
Senior Researcher (SR)								
0454e07f64	4	I	6	0	0	100.00	100.00	100.00
00c32076f4	13	P	8	0	0	100.00	100.00	100.00
0c7d3163ea	9	I	13	1	0	92.86	100.00	96.30
0da5febabf	11	P	8	0	1	100.00	88.89	94.12
0012333581	13	I	11	0	0	100.00	100.00	100.00
0aa1b3161f	5	I	9	0	1	100.00	90.00	94.74
0021fd339f	14	P	4	0	8	100.00	33.33	50.00
039105663f	9	I	11	1	0	91.67	100.00	95.65
02c4f00127	13	P	0	0	3	100.00	0.00	0.00
021c413172	5	I	15	0	0	100.00	100.00	100.00
PhD Student (PS)								
02bf1b3db9	7	I	5	0	2	100.00	71.43	83.33
00b50fc0a8	11	P	2	0	7	100.00	22.22	36.36
02cbc58819	4	I	4	0	3	100.00	57.14	72.73
044939701d	12	P	4	0	2	100.00	66.67	80.00
08e1cb8f4f	16	I	5	1	1	83.33	85.71	84.51
0454e07f64	4	P	0	1	5	0.00	16.67	0.00
00c32076f4	13	I	8	0	0	100.00	100.00	100.00
0c7d3163ea	9	P	9	0	5	100.00	64.29	78.26
0da5febabf	11	I	9	0	0	100.00	100.00	100.00
0012333581	13	P	4	4	3	50.00	72.73	59.26
Master Student (MS)								
0aa1b3161f	5	P	1	0	9	100.00	10.00	18.18
0021fd339f	14	I	12	3	3	80.00	100.00	88.89
039105663f	9	P	4	1	7	80.00	41.67	54.79
02c4f00127	13	I	3	1	1	75.00	100.00	85.71
021c413172	5	P	7	1	7	87.50	53.33	66.27
02bf1b3db9	7	P	2	0	5	100.00	28.57	44.44
00b50fc0a8	11	I	7	2	0	77.78	100.00	87.50
02cbc58819	4	P	5	0	2	100.00	71.43	83.33
044939701d	12	I	5	0	1	100.00	83.33	90.91
08e1cb8f4f	16	P	1	0	6	100.00	14.29	25.00