National Science Library
Chinese Academy of Sciences

A Knowledge Discovery Framework for XML-Literature-Data

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Literature Review

XML-Literature-Data collection:

Scientometric analysis, text information extraction and mining have recently been applied to knowledge discovery using literature data modeled using XML, including publications or patent data. The existing methods proposed some methods using either the paper data or the patent data from XML-data. However, the method of extracting the publications and patent data from the same XML-data file has not been seen.

Different source data mining:

Scientific research and development play important roles in enhancing national competitiveness, so knowledge discovery of literature data becomes a strategic endeavor. These publications or patents data are retrieved from different databases that do not share the same indexing system, which can not allow us to conduct a comparative study at the same level.

Motivation

- CAplus, a database of Chemical Abstracts Service, which is the world’s largest repository of information on chemistry and related publications, provides the XML-data and covers both papers (Types of publications include journal articles, preprints, conference articles, dissertations, and books) and patents in one database.

- One of the merits is that all the data are provided in the same indexing system, including the concepts, substances and roles, commercial or government entity, source of publication, and various other data entities. Thus, the indexing terms can be used to deep mining and make comparisons between the papers and patents.

Motivation

- Our study focuses on the knowledge discovery framework for XML-Literature-Data based on the CAplus database.

- This study presents the methods of text information extraction and text mining on xml-data from CAplus database.

- The integrative use of indexing data on papers and patents of CAplus and the systematic exploration and comparative study of the distribution trends in topics, substance roles, and industrial mapping are distinctive and insightful.

- This study provides a valuable reference for scientists and developers, policy makers, industry and business.

Data Processing Methodology

Data Collection

Data Exploration

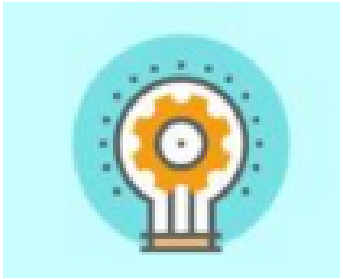
Data Transformation

Run the Java Program to Transform the Data

Data Validation And Verification

Data Cleaning

Featured Data Mining



Knowledge Discovery

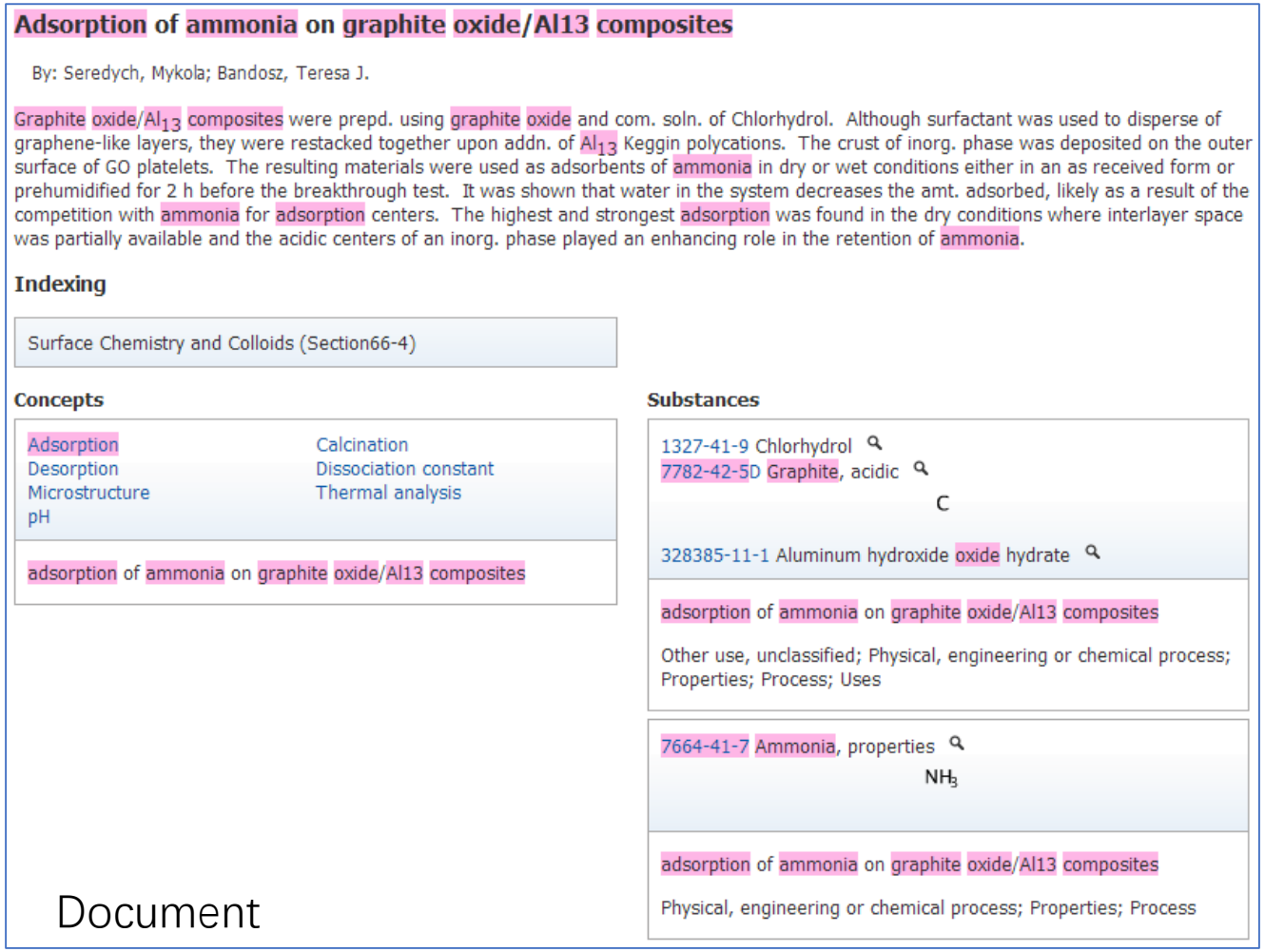
Data Exploration

- **Structure of the data**

  Documents, Indexing, Family,

  Substances, Nomenclature, Keymap

- **Attributes collected:**
  - Title
  - Author
  - Abstract
  - Date
  - Concept
  - Substance



Adsorption of ammonia on graphite oxide/Al13 composites

By: Seredych, Mykola; Bandosz, Teresa J.

Graphite oxide/Al_{13} composites were prepd. using graphite oxide and com. soln. of Chlorhydrol. Although surfactant was used to disperse of graphene-like layers, they were restacked together upon addn. of Al_{13} Keggin polycations. The crust of inorg. phase was deposited on the outer surface of GO platelets. The resulting materials were used as adsorbents of ammonia in dry or wet conditions either in an as received form or prehumidified for 2 h before the breakthrough test. It was shown that water in the system decreases the amt. adsorbed, likely as a result of the competition with ammonia for adsorption centers. The highest and strongest adsorption was found in the dry conditions where interlayer space was partially available and the acidic centers of an inorg. phase played an enhancing role in the retention of ammonia.

Indexing

Surface Chemistry and Colloids (Section66-4)

Concepts

Adsorption
Calcination
Desorption
Dissociation constant
Microstructure
Thermal analysis
pH

adsorption of ammonia on graphite oxide/Al13 composites

Substances

1327-41-9 Chlorhydrol
7782-42-5D Graphite, acidic
C

328385-11-1 Aluminum hydroxide oxide hydrate

adsorption of ammonia on graphite oxide/Al13 composites

Other use, unclassified; Physical, engineering or chemical process; Properties; Process; Uses

7664-41-7 Ammonia, properties
NH_3

adsorption of ammonia on graphite oxide/Al13 composites

Physical, engineering or chemical process; Properties; Process

Document

Data Transformation

- **Keymap analysis:**

Analysis of document centric key map between all documents and any associated indexing.

- **Reclassification:**

Each file contains one document and associated indexing files, and separates the papers from the patents.

- **Data extraction:**

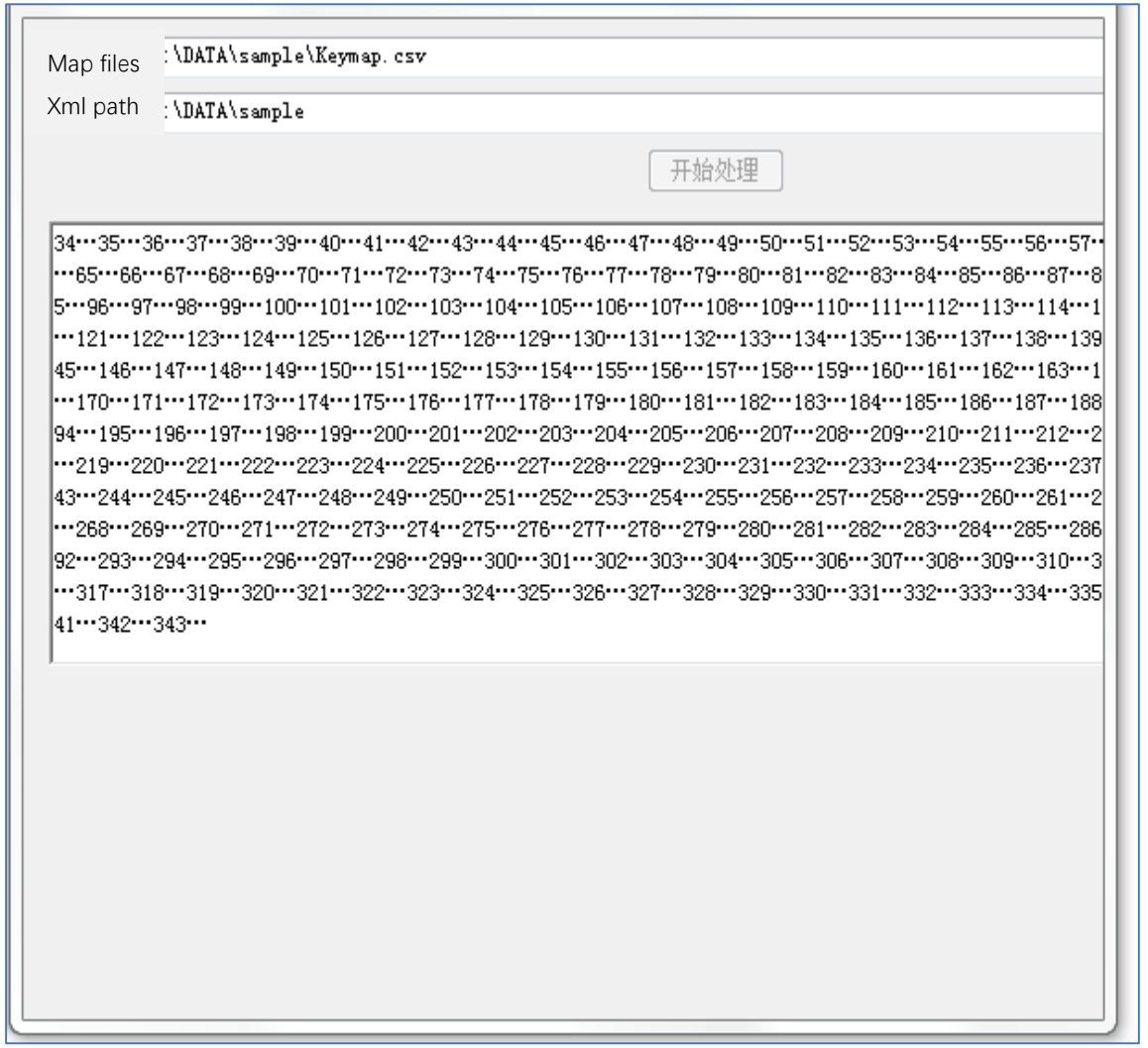
Extraction for each attribute for papers and patents.

- **Output:**

Comma-Separated Values

- **Challenge:**

Substances need to match its function.



Data Cleaning and Statistics

- **Data Cleaning:**

Remove noise and merge different spelling of one entity.

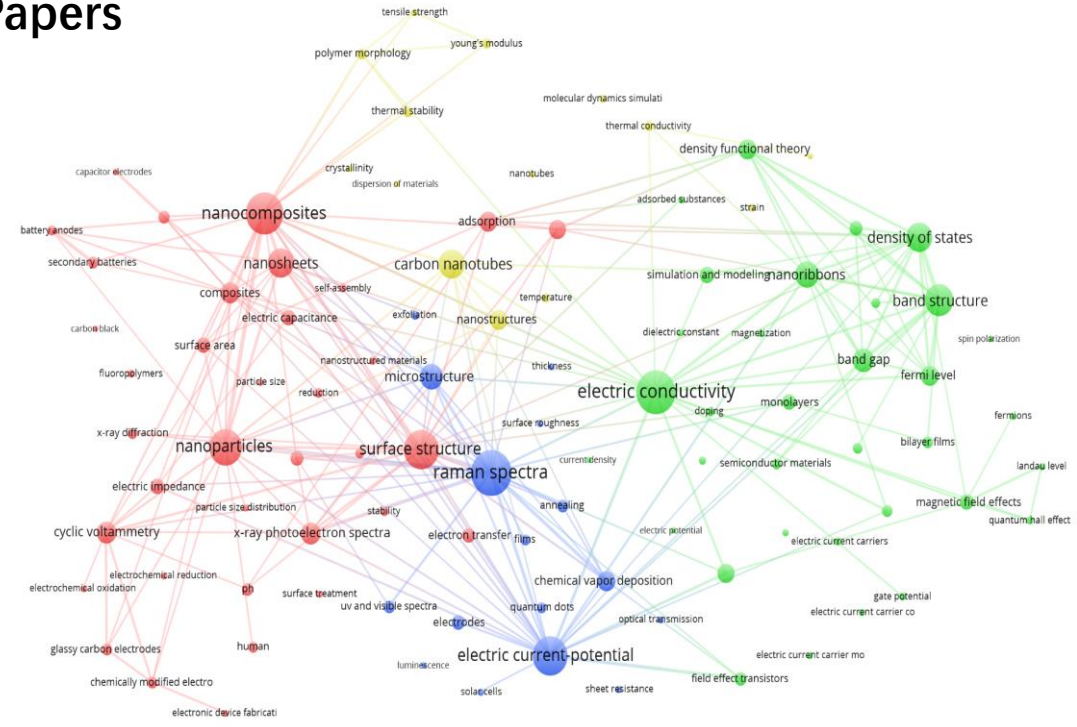
- **A case study: Global Graphene Research**

- **Data statistics:**

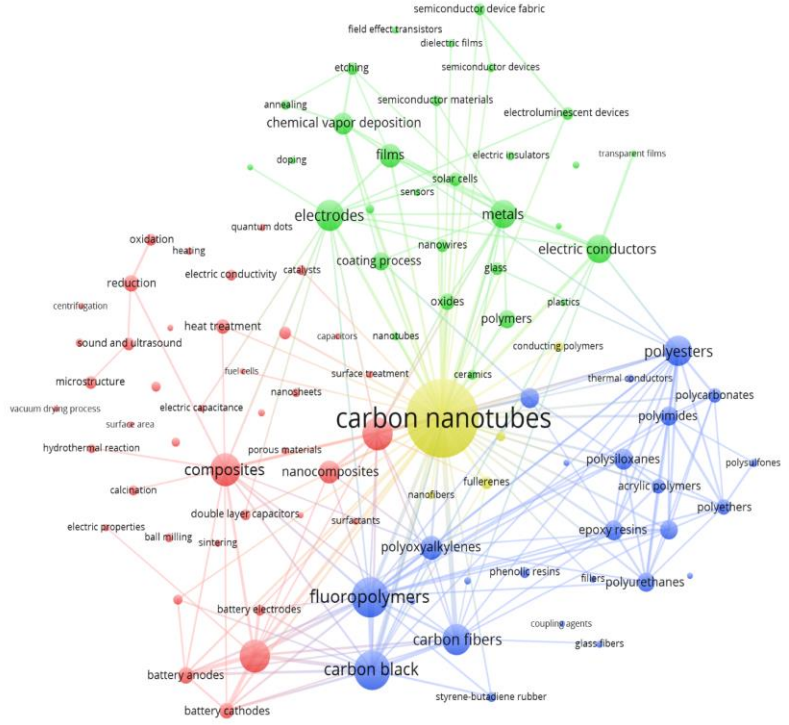
– 78756 papers, 23057 patents ,which covered all years
– 9424 concepts in papers, 8471 concepts in patents
– 19413 substances in papers, 27568 substances in patents
– Publication year range: 1985-2017 for papers, 1997-2017 for patents

Concepts and Topic Clustering

Papers



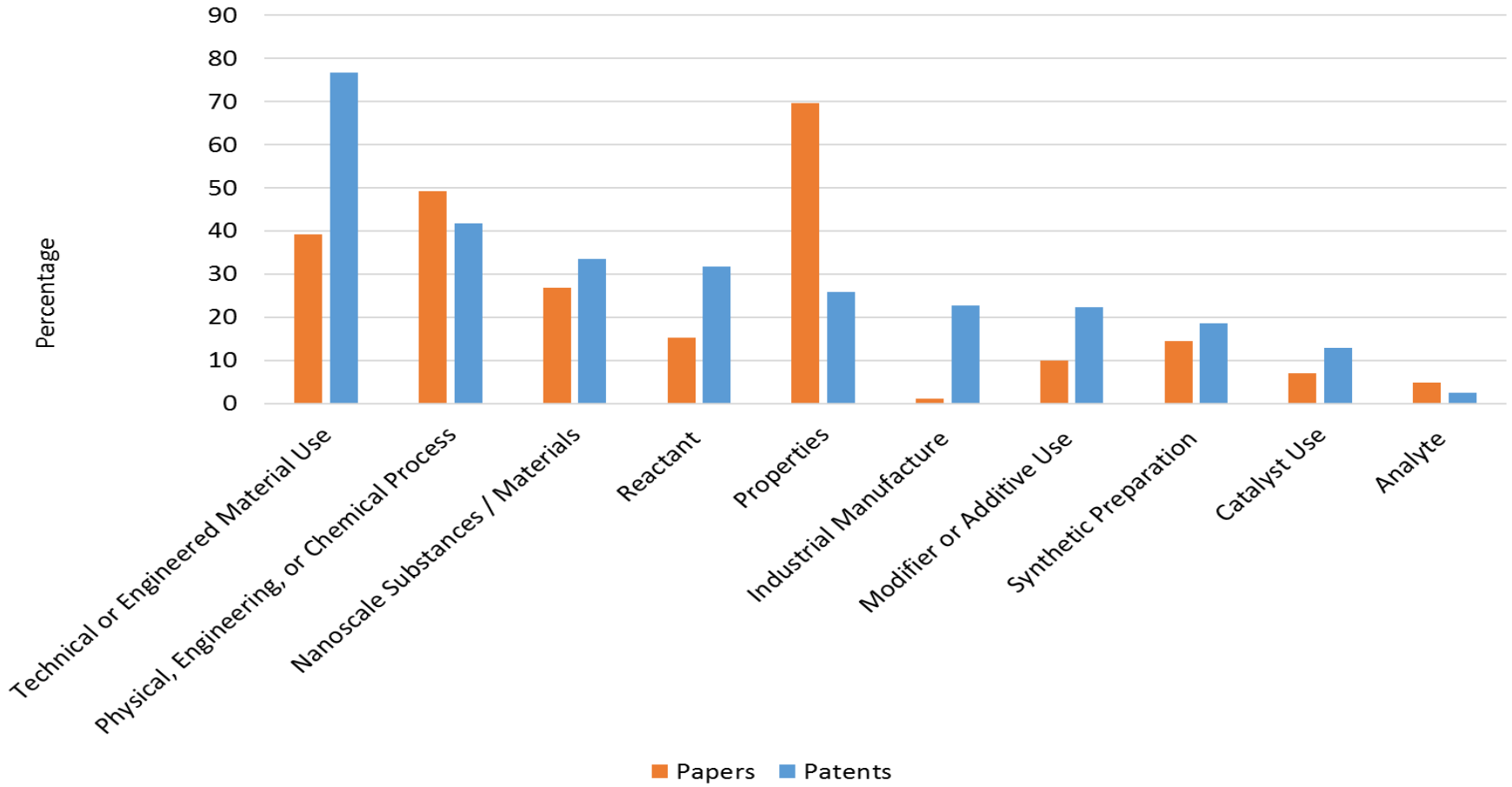
Patents



Differences of topic clustering between papers and patents

The concepts clustering presents the difference that the research fields of papers focus on the fundamental research, such as material structure and electrical properties, while the patents show the hot topics of application fields, such as batteries, semiconductors.

Substances and roles

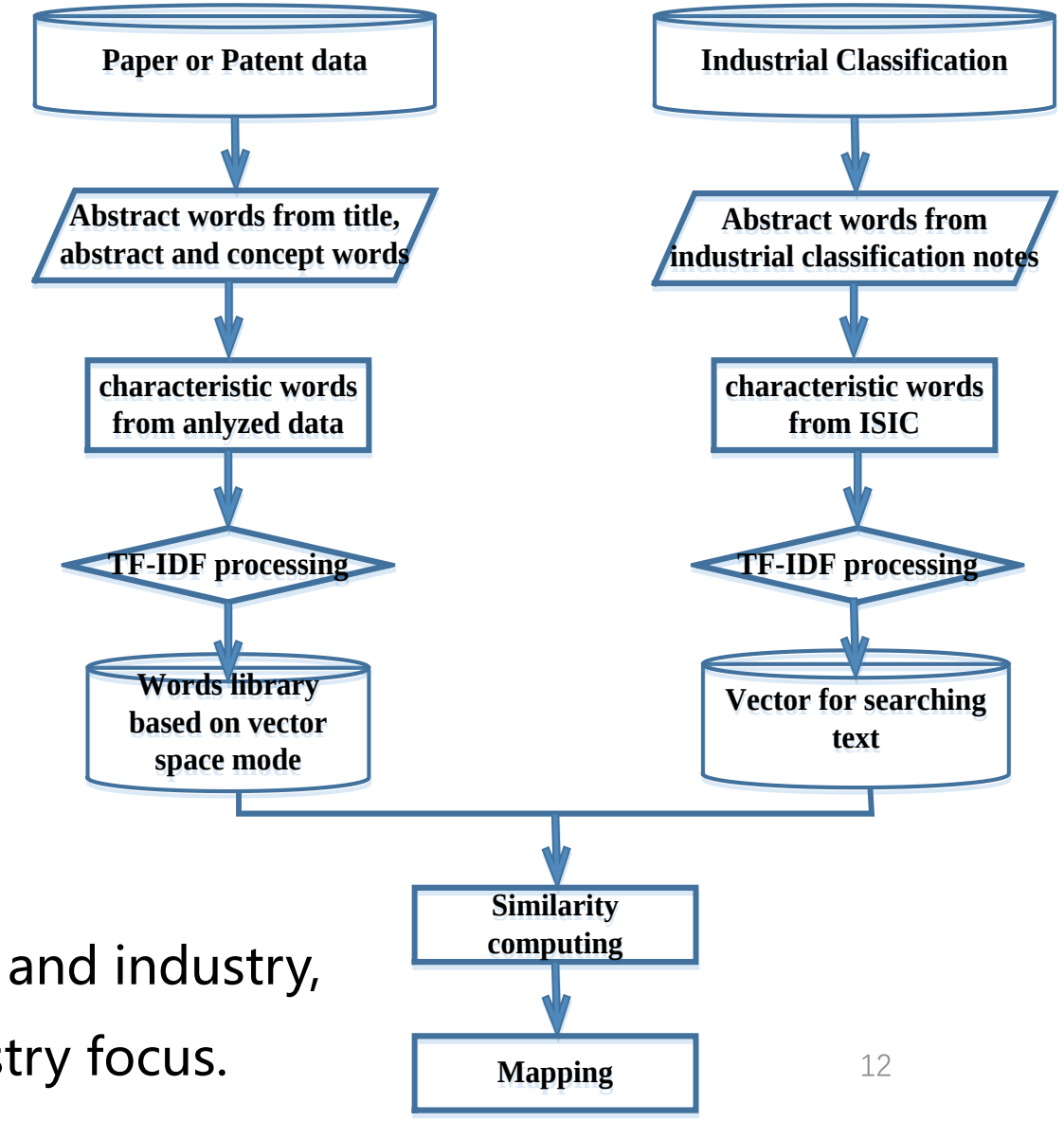


Different roles of substances in papers and patents

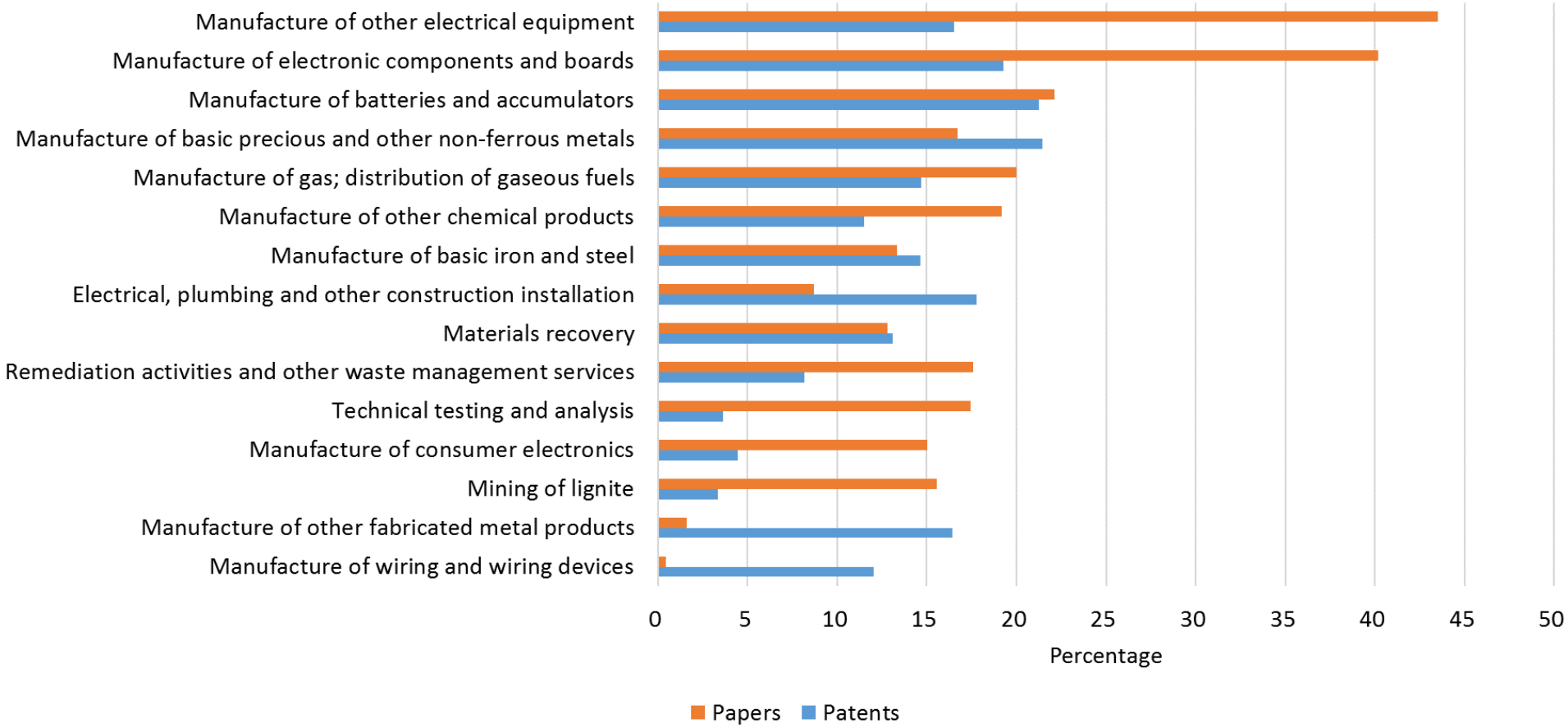
The roles of substances in papers are related to properties, while the patents focus more on the technical or engineered material use, industrial manufacture or additive use.

Link scientific research to industry

- **Data extraction and processing**
  - Title, abstract, concepts in papers or patents
  - Terms of industrial classification from International Standard Industrial Classification of all economic activities (ISIC)
  - Term Frequency - Inverse Document Frequency （TF-IDF） processing
- **Data mining**
  - Cosine similarity computing
  - Determine the threshold
  - Find the relationship between scientific research and industry, industry coverage, economic activities and industry focus.



Link scientific research to industry



Industrial mapping of papers and patents

The papers are linked to the industrial classification, such as the electrical equipment, the consumer electronics, on contrast, few patents are linked to these areas.

Conclusion

- We introduced literature research methods in knowledge discovery and proposed a knowledge discovery framework for XML-literature-data, which tailored for the CAplus database.

- We designed a customized tool for the CAplus data transformation, and XML data files were mapped into an internal processing file format.

- We presented the data mining methods to indicate the differences between the fundamental research and technology development, based on the same indexing system.

Future Work

- The customized tool that extracts the citation data.

- Add literature data mining methods:
  - Citation network analysis
  - Topic modeling for concepts
  - Deeper mining for substances and roles

- To study and understand the relationship between the fundamental research and technology development

References

- Consoli, S. and Stilianakis N. I.. A quartet method based on variable neighborhood search for biomedical literature extraction and clustering. International Transactions in Operational Research., 2017, 24(3), 537–558.
- Eck, N.J.V., Waltman, L. Text mining and visualization using VOSviewer. ISSI Newsletter, 2011, 7(3), 50–54.
- Eck, N.J.V., Waltman, L. How to normalize cooccurrence data? An analysis of some well-known similarity measures. Journal of the American society for information science and technology, 2009, 60(8), 1635–1651.
- Jessop, D.M., Adams, S.E., Murray-Rust P. Mining chemical information from open patents. Journal Of Cheminformatics, 2011, 3(1), 40.
- Klincewicz, K.. The emergen t dynamics of a technological research topic: The case of graphene. Scientometrics, 2016, 106(1), 319–345.
- Le, S.S., Polytechnic, N. Technological innovation trend of graphene technology: A research based on the patentometric analysis. World nonferrous metals, 2017(9), 94–95.
- Lee, K., Kim, B., Choi, Y., et al. Deep learning of mutation-gene-drug relations from the literature. BMC bioinformatics, 2018, 19(1), 21.
- Lee, K., Shin, W. , Kim, B., et al. Translated PubMed and PMC texts to networks for knowledge discovery. Bioinformatics, 2016, 32(18), 2886-2888.
- Zhao Z.X., Chen H. Development of graphane technology in China: Present and future—based on patent statistics. China Textile Leader, 2016(9), 40–43.
- Zheng J. Comparative analysis of research paper and high level research paper of graphene field. Advanced materials industry, 2016(10), 48–51.

Thank you!

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