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Materials Synthesis Insights from Scientific Literature via Text Extraction and Machine Learning

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Background

Background

Why This Matters: The Need for Data-Driven Synthesis

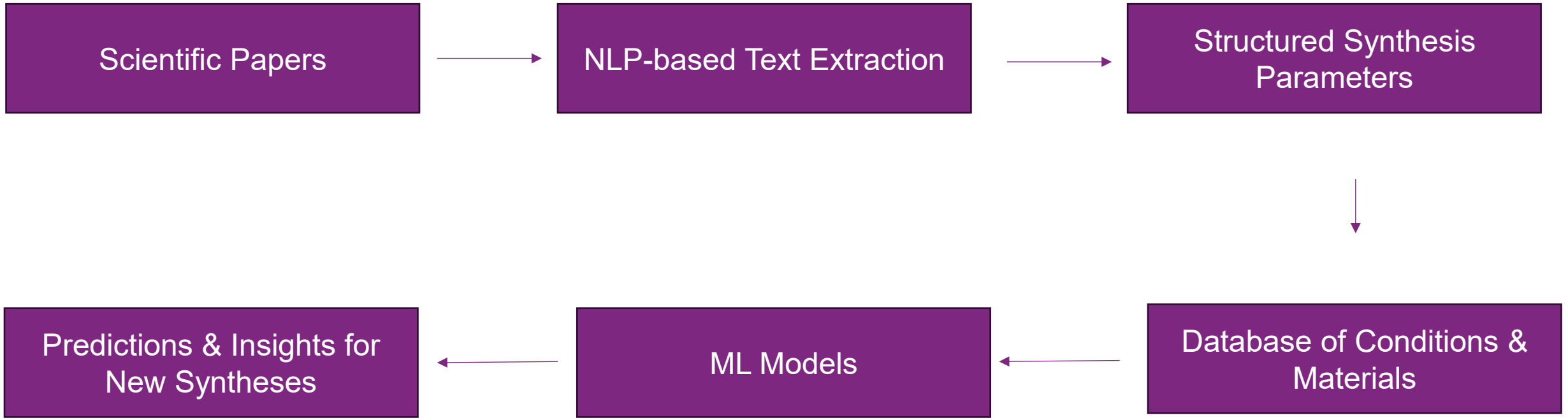
- The pace of discovering new materials is often slowed by the lack of efficient synthesis strategies.
- Traditionally, synthesis relies on heuristics, which do not scale with the rapid growth of computational material predictions
- This project leverages **Natural Language Processing (NLP)** and **Machine Learning (ML)** to extract and analyze synthesis parameters from thousands of published scientific articles.

By building a large, structured database of synthesis conditions, we can:

- Understand key parameters influencing material properties
- Improve reproducibility and guide new syntheses
- Enable data-driven automation in materials design

Background

Framework for Literature-Based Synthesis Extraction



Methodology

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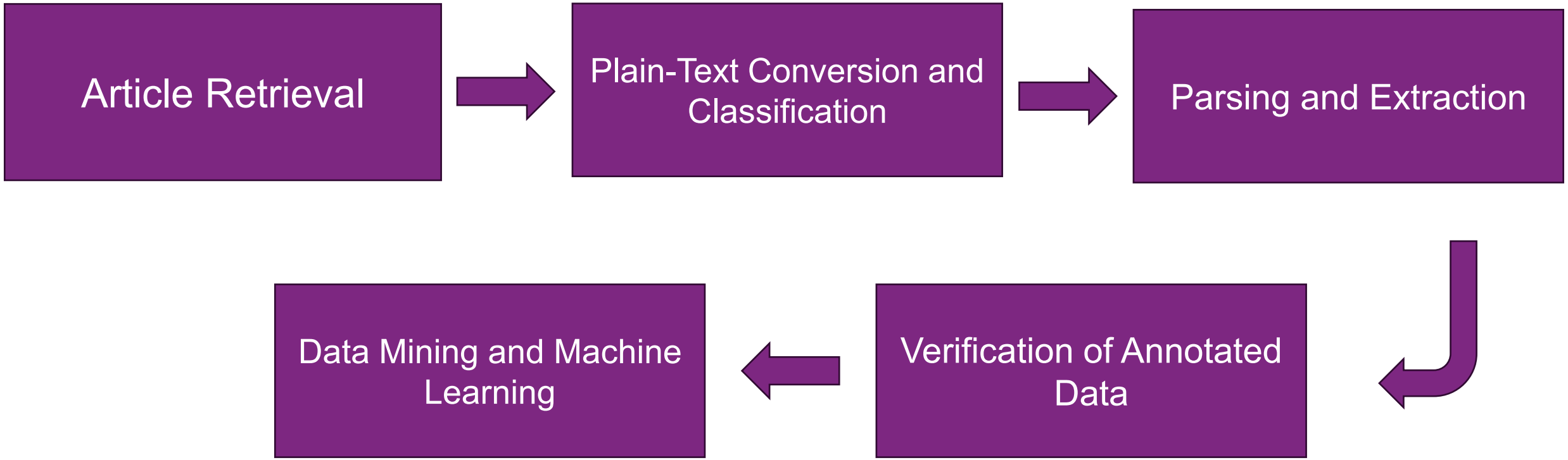

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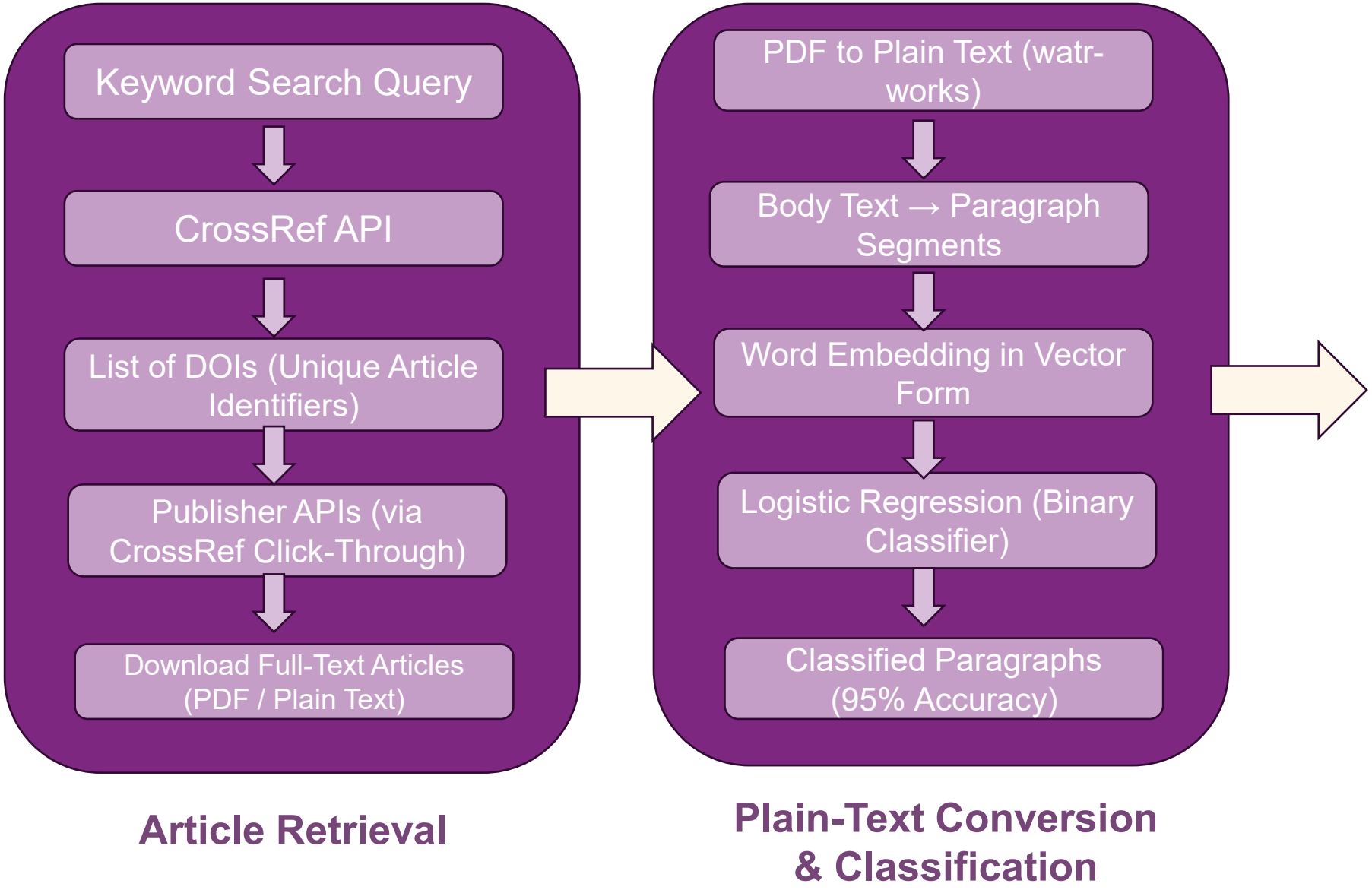
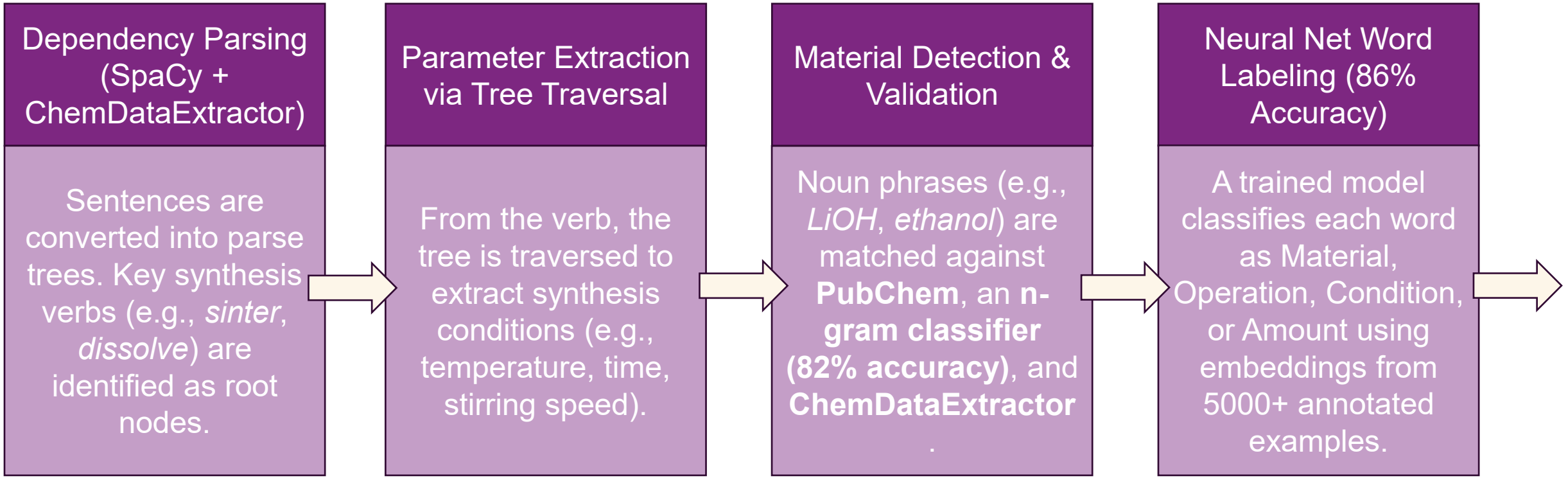
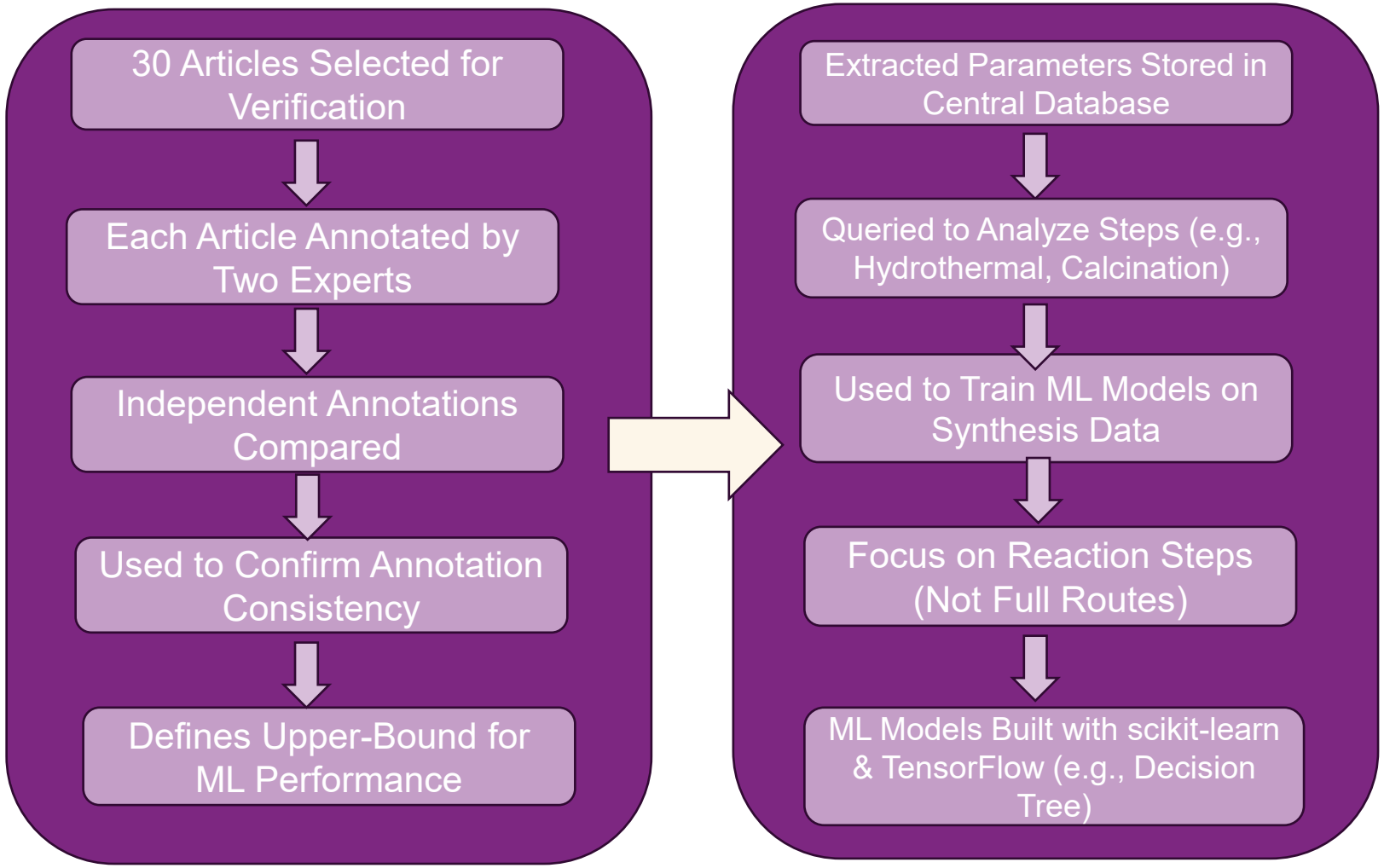


Methodology



Parsing and Extraction

Methodology

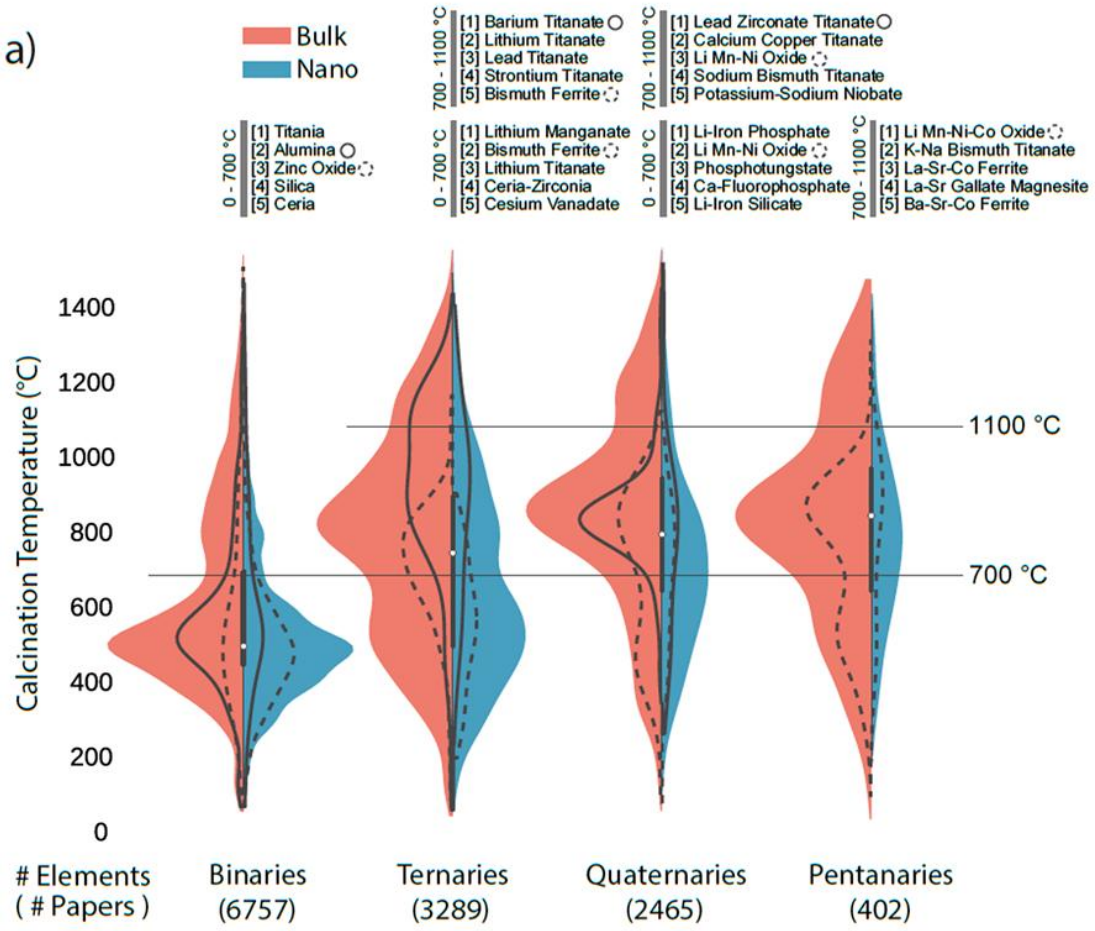


Verification of Annotated Data

Data Mining and Machine Learning

Results

Results



Calcination Temperature Distribution Across Metal Oxide Systems (Bulk vs Nano)

Bulk vs Nano Trend:
Bulk materials are typically calcined at **higher temperatures** than their nanostructured counterparts.

Complexity Increases Temperature:
Calcination temperature increases with **elemental complexity,** from binaries to pentanaries, especially in **nano** syntheses.

Binary Oxide Range:
Most binary oxides fall between **450–550 ° C**

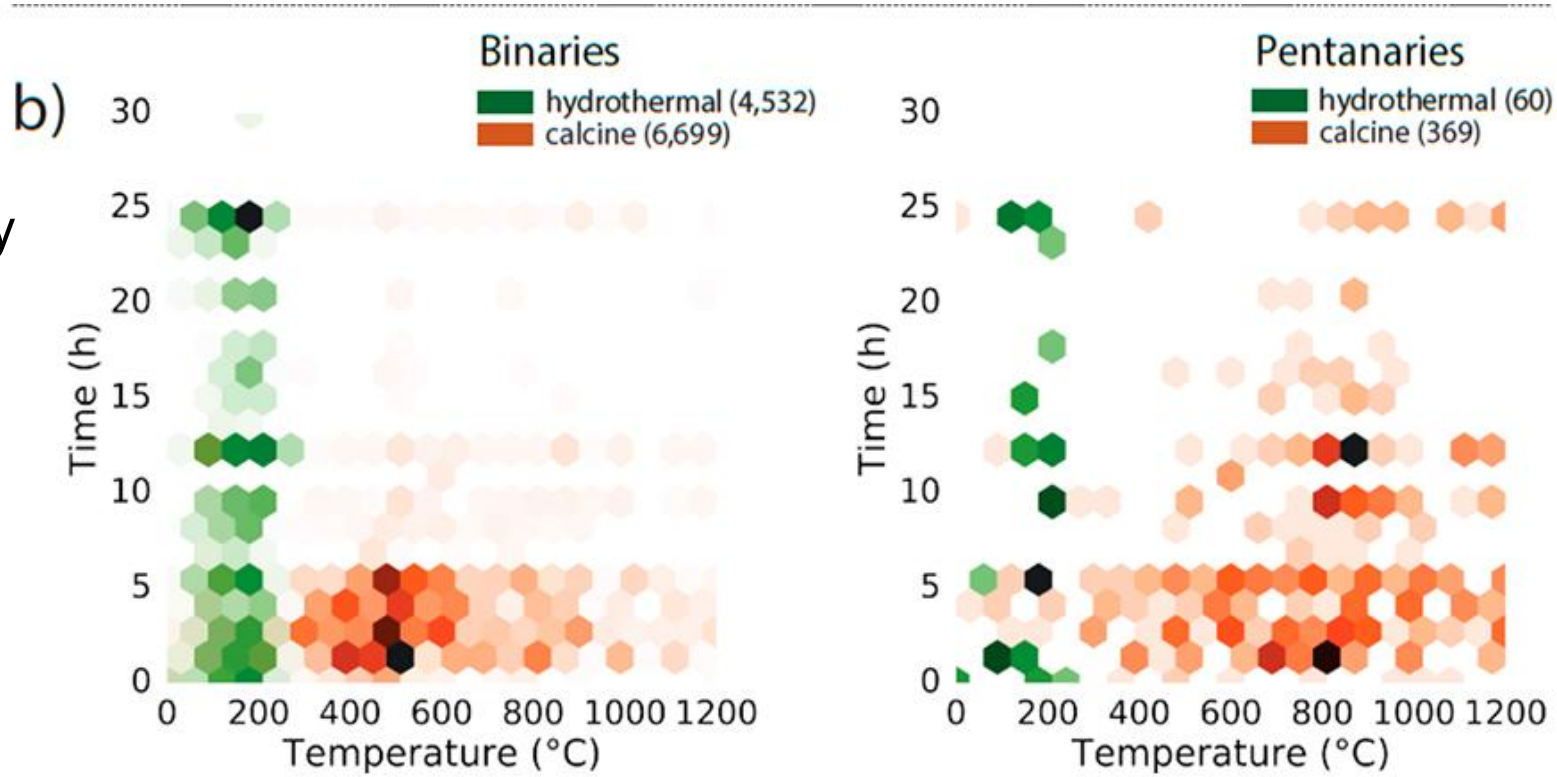
- **Alumina:** found more in bulk
- **ZnO:** more in nano form

Ternary oxide Range:

- **Bismuth Ferrite:** sharp peak at 750 ° c(bulk) and around 600 ° C for nano.
- **Barium Titanate:** wider range, 900-1100 ° C

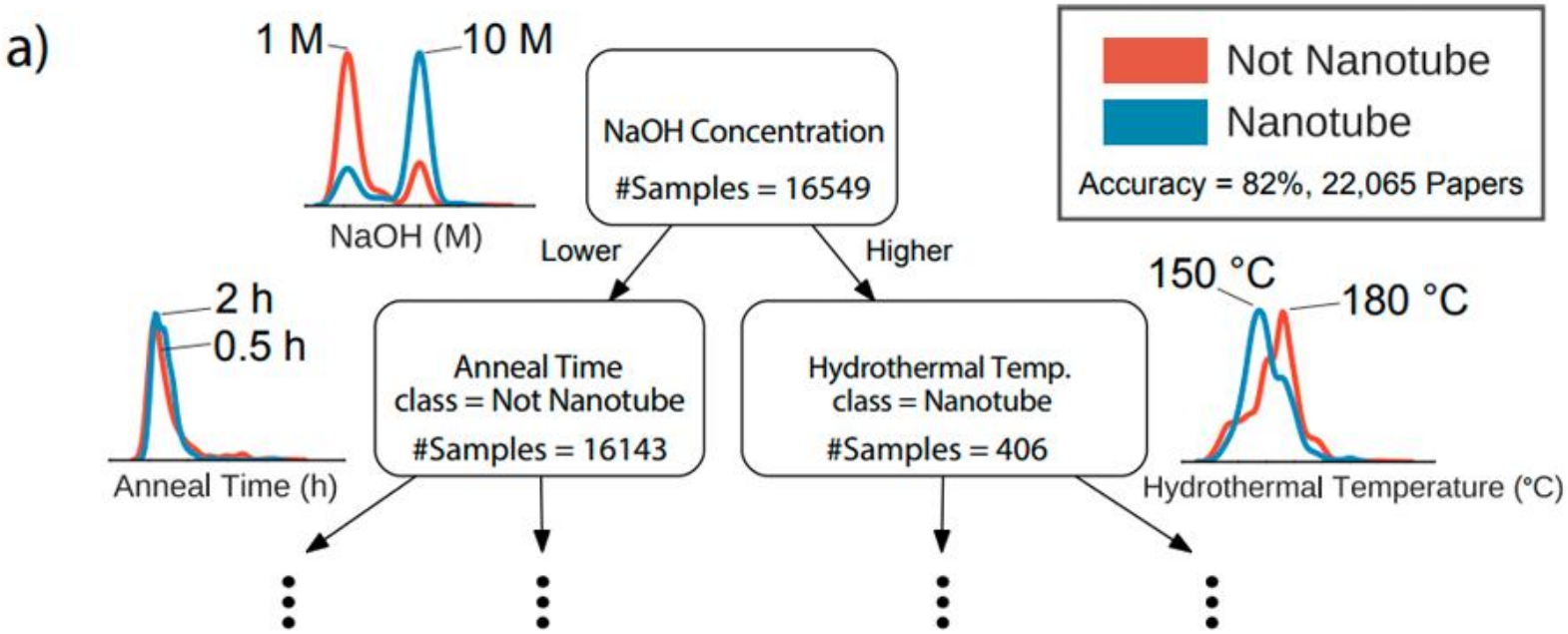
Results

- **Hydrothermal reactions** occur at **low temperatures** (typically 150–200 °C) and **long durations** (12–24 hours).
- Reaction temperatures are limited by the **critical point of common solvents** (e.g., water, ethanol).
- **Calcination steps** happen at **much higher temperatures** and usually **shorter times**.
- As material complexity increases, **calcination temperatures and durations both rise**.
- Simple systems concentrate around **400–500 °C, <5 h**, while complex ones extend to **800–900 °C, >5 h**.



Temperature–Time Distribution of Hydrothermal and Calcination Syntheses

Results



Decision Tree for Titania Nanotube Formation

Key Features Identified:

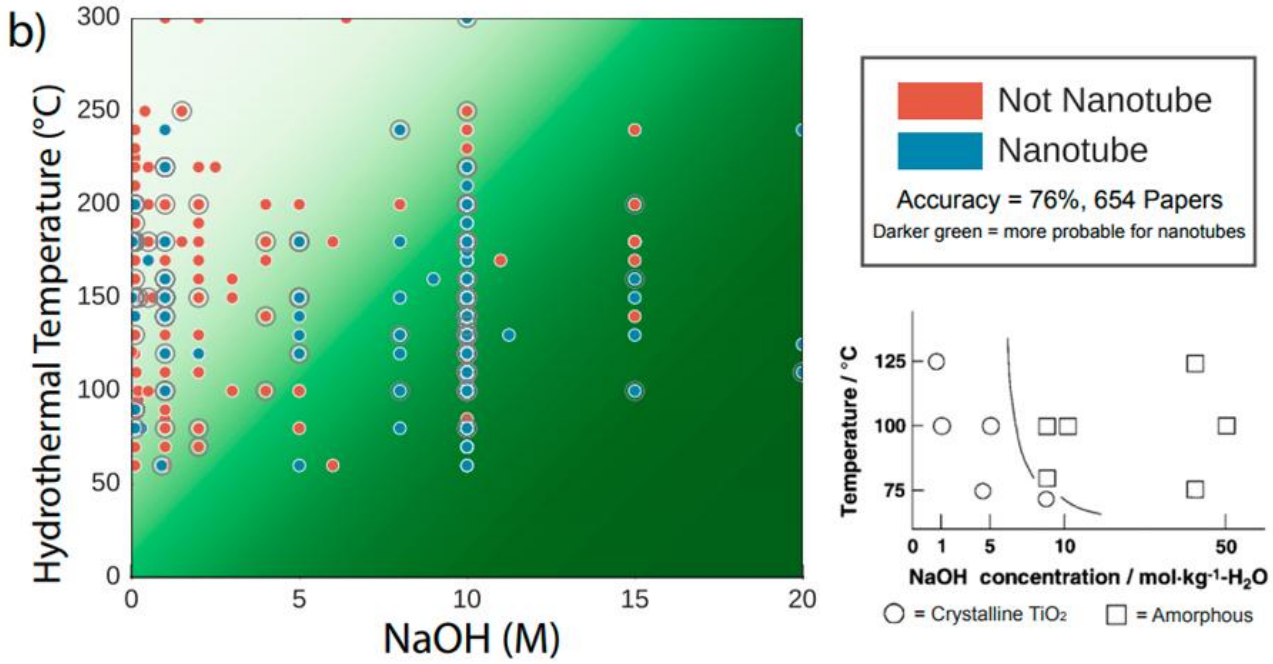
NaOH concentration (most important , root node)
is commonly clustered around **1 M and 10 M**

Hydrothermal temperature also plays a significant role
Some notable peaks at **150° C and 180° C**

Annealing time was found to be **less predictive**, as its values didn't clearly distinguish between outcomes.

The model achieves 82% classification accuracy, showing that NaOH concentration and hydrothermal temperature are strong indicators of nanotube formation.

Results



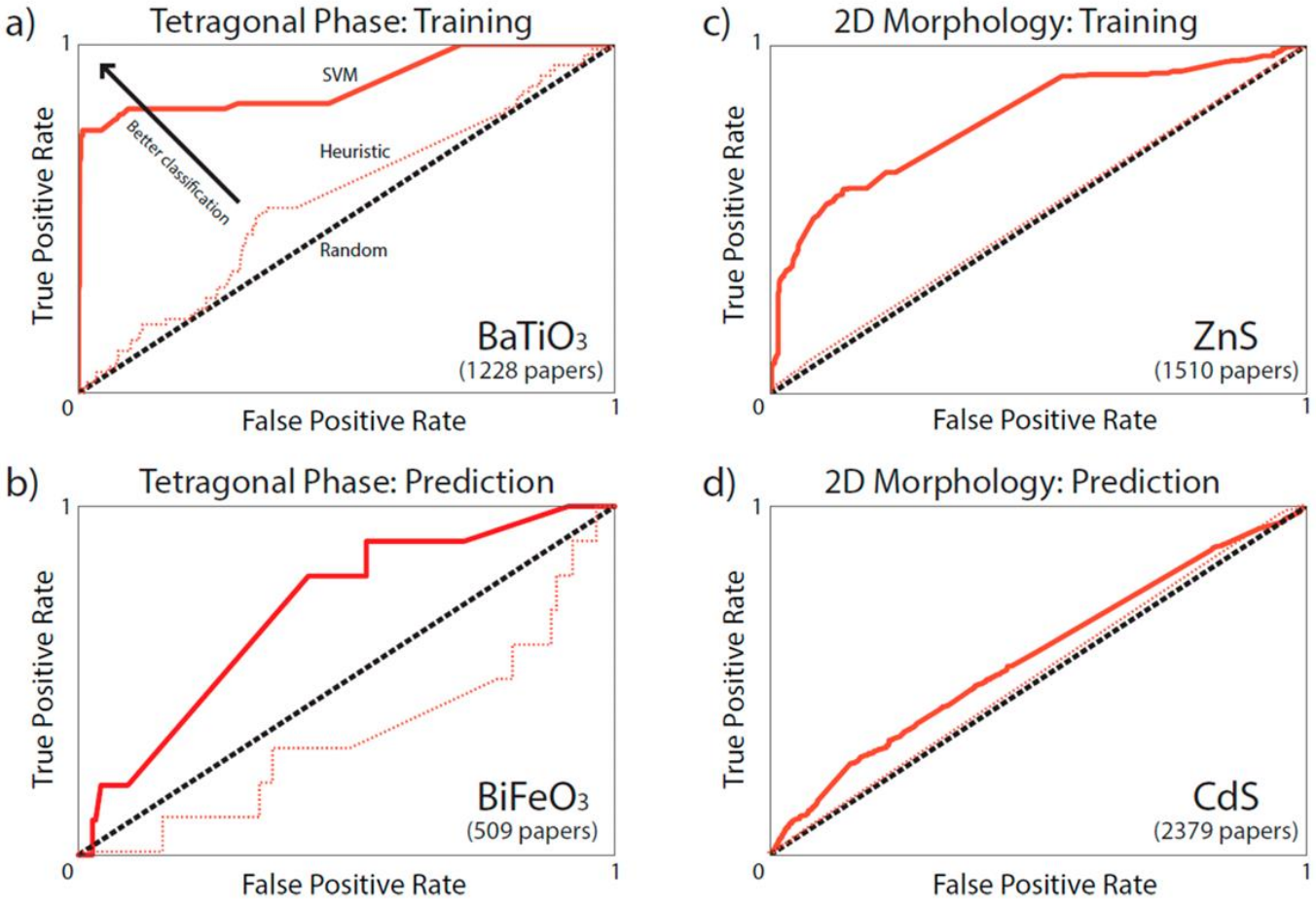
Machine-Learned Phase Diagram for Titania Nanotube Formation

The diagram shows higher probability of nanotube formation (darker green) at:

- High NaOH concentrations
- Lower hydrothermal temperatures

This reduced parameter space allows for easy visualization of synthesis trends using only experimentally accessible variables.

Results



Machine-learned classifiers and predictions across materials systems

All four subfigures compare three models:

– **Support Vector Machine (SVM)** with Gaussian kernel

– **Heuristic (simple rule-based)**

– **Random guessing**

SVM consistently outperforms both the heuristic and random strategies.

Demonstrate **robustness and transferability of machine learning models** across materials and synthesis outcomes.

Conclusion

Conclusion

This work bridges the gap between published knowledge and predictive synthesis planning.

Built an **automated framework** to extract synthesis data using **text mining and ML**.

Compiled a **large-scale database** of synthesis conditions from scientific literature.

Identified **key parameters** (e.g., temp, time, solvent) that influence material outcomes.

Enabled **accurate predictions** without prior domain knowledge or manual input.

Future Outlook

Future Outlook

Extend coverage to more synthesis methods

Thin film deposition, catalytic systems, non-crystalline materials

Refine data accuracy

Weighting **highly cited papers**
Incorporating **newly published research**

Thank You

Any Questions?