Synthesis of cuprate superconductors predicted from a closed loop machine learning model to accelerate materials discovery

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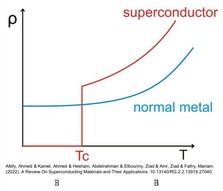
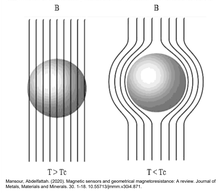
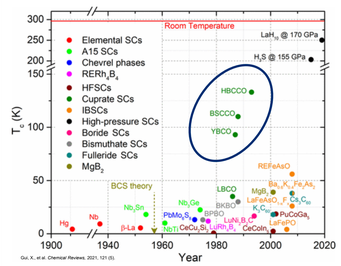
Superconductivity



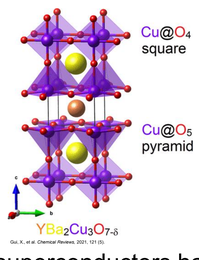
Below a critical temperature (T_C), superconductors:
- conduct electrical current with **zero resistance**
- **expel magnetic fields**



Applications:
- Electric power generation & transmission
- MRI devices
- Maglev transportation
- Quantum computing



Applications are limited due to **low critical temperatures**, requiring liquid He or liquid N to cool to superconducting state.



Cuprate superconductors have the highest T_C at ambient pressure. Properties of the copper oxide (CuO_2) layers are theorized to be the mechanisms for superconductivity.

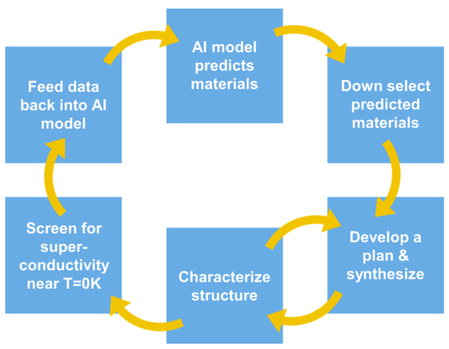
Closed loop machine learning

Is generative AI a useful tool to advance materials discovery?

Can AI predict specific properties of materials?

Can the model be improved via experimental data?

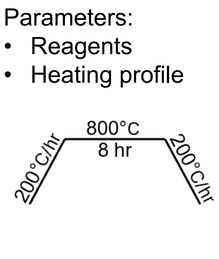
- Synthesize AI predicted high temperature superconductors in cuprate family
- Characterize phases that formed
- Feed raw data and human interpretation back into model
- Improve future predictions



Synthesis methods

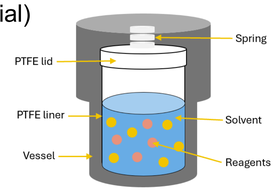
Solid state synthesis

Parameters:
- Reagents
- Heating profile



Hydrothermal synthesis

Parameters:
- Reagents (acidity, solubility, oxidizing potential)
- Heating profile
- Pressure



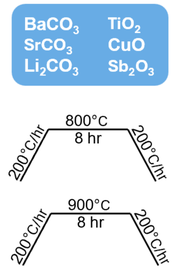
Other synthesis techniques include molten salt flux, chemical vapor transport, floating zone, etc.

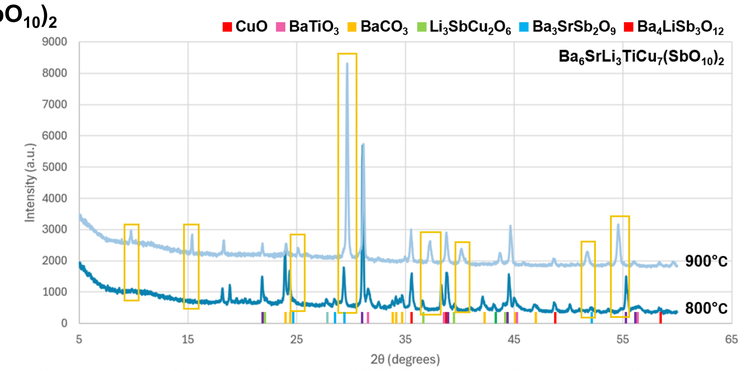
Results

Several of the many predicted and synthesized materials show **unknown patterns** in the PXRD scan. Presented below is one such result.

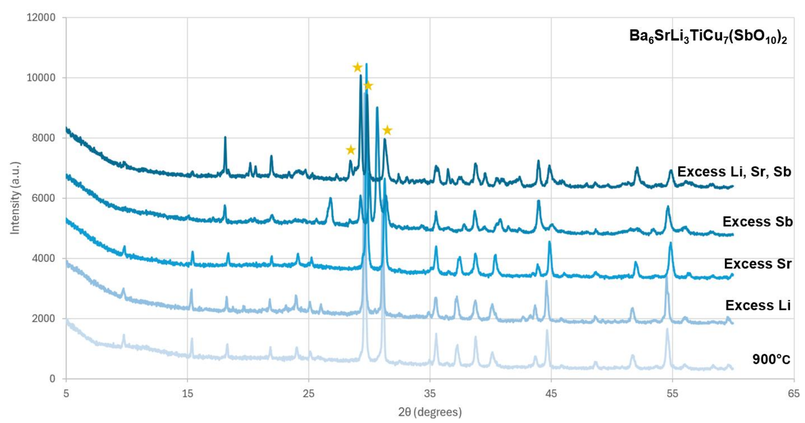
$Ba_6SrLi_3TiCu_7(SbO_{10})_2$

$BaCO_3$	TiO_2
$SrCO_3$	CuO
Li_2CO_3	Sb_2O_3





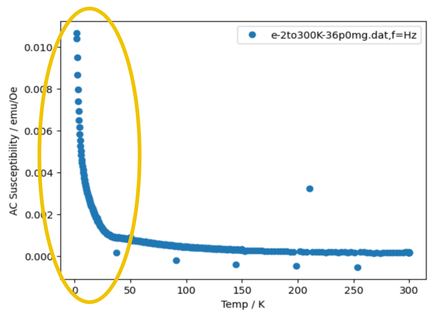
CuO and $BaTiO_3$ are the only identified patterns in 900°C sample. Thus, strontium, lithium, and antimony are likely present in majority phase unknown (yellow rectangles).



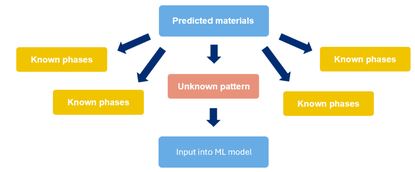
Attempt to isolate unknown peaks by tuning stoichiometric ratios of reagents. Excess antimony alters pattern. Excess lithium and strontium preserve the unknown peaks.

Superconductivity results

No superconducting results were found for the predicted and synthesized compounds. Superconductivity is indicated by a sharp downward slope as the temperature approaches 0K.



Conclusion



Lack of knowledge about superconducting mechanisms makes the realization of novel high temperature superconductors challenging. Generative AI, in combination with experimental data, could advance the discovery of materials hosting specific, advantageous properties. Despite not finding any superconducting results, several possibly new phases have been synthesized based on AI prediction.

Future Work

Continuing to isolate unknown peaks of interesting compounds to synthesize phase pure samples, of which superconductivity test can be run and crystals can be made.

Repeating similar procedures on future material predictions to train the ML model and improve predictive power.

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