Synthesizing AI-Predicted Cuprate Superconductors

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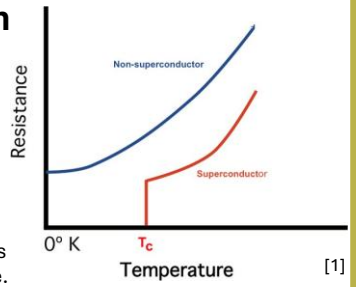
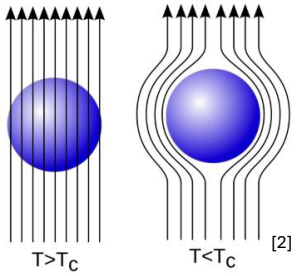
Introduction

Superconductors (SC) conduct electricity without resistance below their critical temperature (T_c). T_c is often very low (~0-10 K), which makes using most superconductors difficult and expensive.



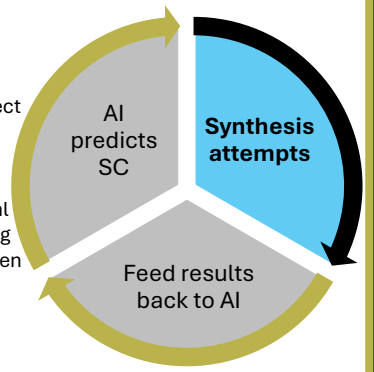
[1]



[2]

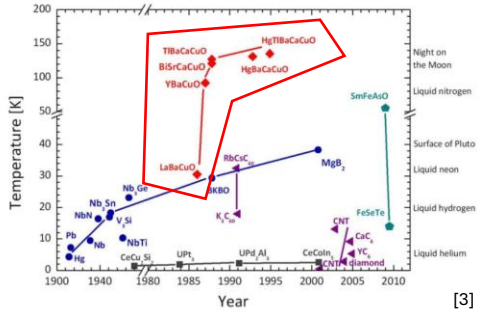
Below their T_c, superconductors expel magnetic fields, which enables superconductivity to be easily measured.

The goal of this project was to synthesize cuprate superconductors predicted by artificial intelligence (AI) using solid-state and molten salt flux syntheses,



Cuprate Superconductors

- Cuprates are copper oxides
- Relatively high temperature superconductors
- Examples shown in red.



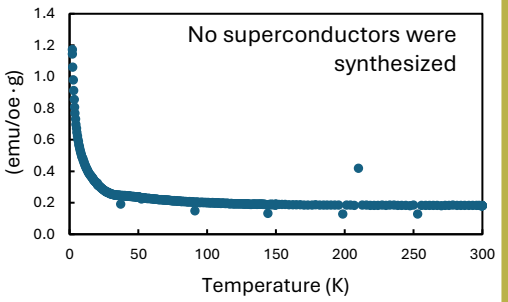
[3]

Solid State Synthesis Results

Grind, transfer to crucible → Heat ~900 °C

= Metal oxides/carbonates = Products

Ba4Sr4Li2TiCu9O20	LiLa2TiCu3PbO9	BaLiCu2(PbO3)2	SrLaCu2Bi2O7
Ba4Sr2Li2TiCu7O16	SrLi2Cu4Bi2PbO10	SrLa2YTiCu3O10	SrTiCuPb5O9
Ba4Sr2Li3TiCu9PbO19	Li2Cu5CO8	Sr2YCu4PbO9	Li2YCu5Sn2Pb2O13
Ba2SrLi2Ti4Cu8Bi2PbO24	LaCuO3	LiYCu4Sb2O9	BaTi2Cu2Pb3O10
Ba2Sr5Li2TiCu9PbO20	SrLiMg2Ti(CuO2)5	BaSrLi2Cu4O7	BaNd(CuO2)2
BaLi2Cu4SnBi2O11	LiCuSnBiO5	YCu8Sn2PbO14	BaSr2Li(CuO2)4
Cu3SnPbO6	LaYCu4Pb4O11	BaSrYTiCu2O7	La2YTiCu3PbO10



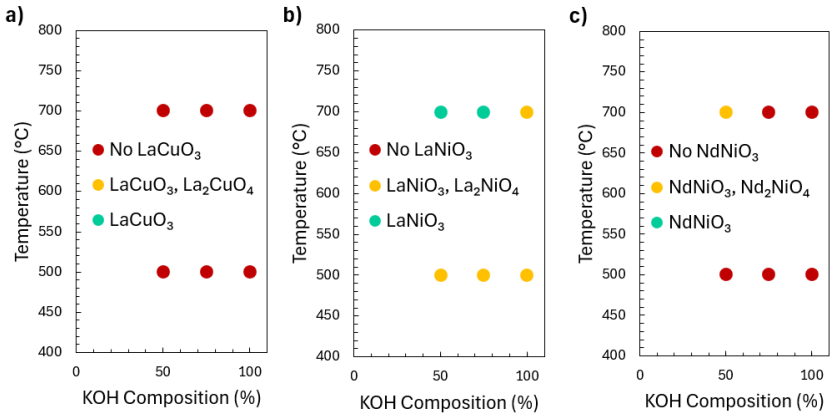
- All targeted cuprates shown (left)
- highlighted = unknown phase detected
- Isolation ongoing

Molten Salt Flux Results

KOH – KI flux mixture
1:1, 3:1, & 1:0 KOH:KI ratios
500 °C, 700 °C

a) $LaCuO_3$ (target)
b) $LaNiO_3$ (indicator)
c) $NdNiO_3$ (indicator)

Higher temperature, higher KI concentration better for oxidation



Conclusions & Future Work

AI predictions were used to target novel cuprate superconductors, which were synthesized using both solid-state and molten salt flux methods. While no superconductivity was observed in the synthesized products, several previously unreported phases were produced. Molten salt flux synthesis, though unsuccessful in yielding the target compound, provided useful insight into the oxidizing capabilities of KOH-KI fluxes. Further work should be conducted to isolate novel compounds and to explore the KOH-KI phase space for optimizing oxidation.

References

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