Discovery of Novel Superconducting Materials with Deep Learning

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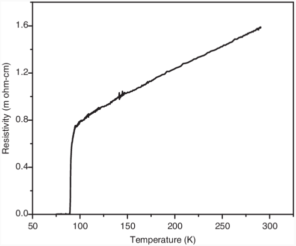
Baylor University

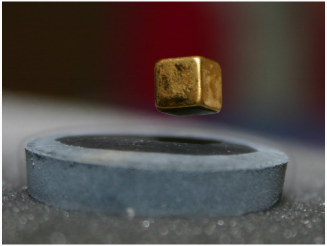
Background

Superconductors

- Superconductors are materials that exhibit two key properties at low temperatures:
  1. The resistivity ρ drops to 0Ω (Current flows without resistance).
  2. Magnetic fields are expelled in the bulk. (Meissner Effect)

Example: $YBa_2Cu_3O_{7-\delta}$ [VBRS14]





- A superconductor's critical temperature (T_c) is the highest temperature at which it exhibits these two properties.

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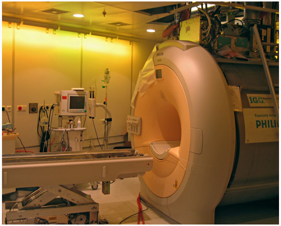
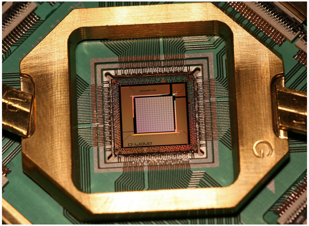
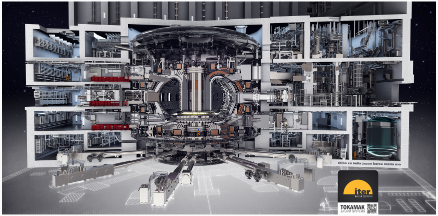
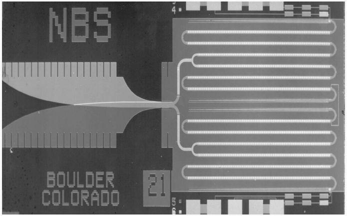
Industrial Applications of Superconductors









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Superconductors

- Superconductivity occurs due to anomalous quantum mechanical pairing of electrons [Coo60].
- Pairing allows for condensation of conducting electrons into a single energy state at the Fermi level, E_F:

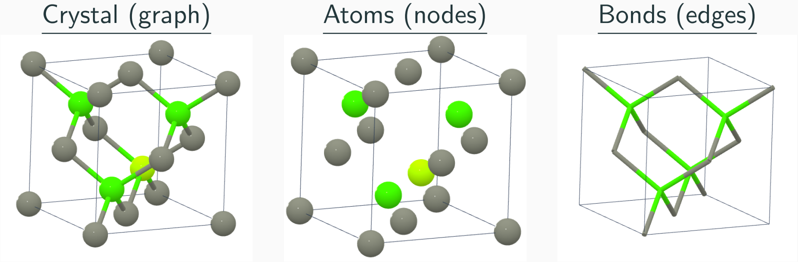
$$\underbrace{|\uparrow\rangle, |\downarrow\rangle}_{\text{Spin-1/2 electrons}} \longrightarrow \underbrace{\frac{(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)}{\sqrt{2}}}_{\text{Spin-0 Singlet Cooper pair}}$$

$$\underbrace{|\uparrow\rangle, |\uparrow\rangle}_{\text{Spin-1/2 electrons}} \longrightarrow \underbrace{|\downarrow\downarrow\rangle, \quad \frac{(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)}{\sqrt{2}}, \quad |\uparrow\uparrow\rangle}_{\text{Spin-1 Triplet Cooper pairs}} \quad [\text{m} = \text{-1, 0, +1}]$$

- Pairing in conventional (i.e. BCS) superconductors is mediated by phonons [BCS57].
- Pairing in unconventional superconductors has not yet been fully explained [ZLI+21].

Alternative Methods for Predicting T_c

- There has been great interest in applying machine learning to superconductor discovery (e.g. see: [SOK+18][KKN+21][XQH+22])
- Very few of these approaches directly incorporate atomic structure (e.g. [CG22]).
- Crystalline structures are naturally interpreted as periodic graphs:



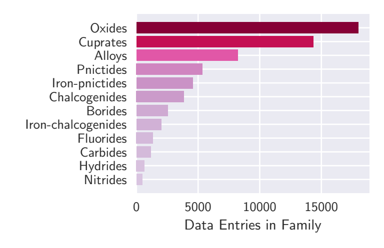
- In this work, we applied graph neural networks to identify superconductors and predict T_c from raw crystalline structure.

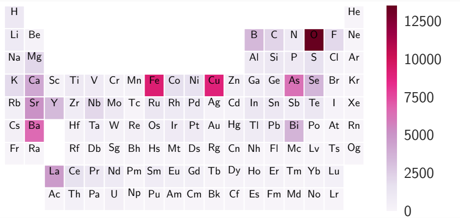
Methods

Data Sources

- We combined two large experimental measurement datasets (*Supercon v1* [SOK+18] and *Supercon v2* [FdCS+23]).

Dataset Distribution

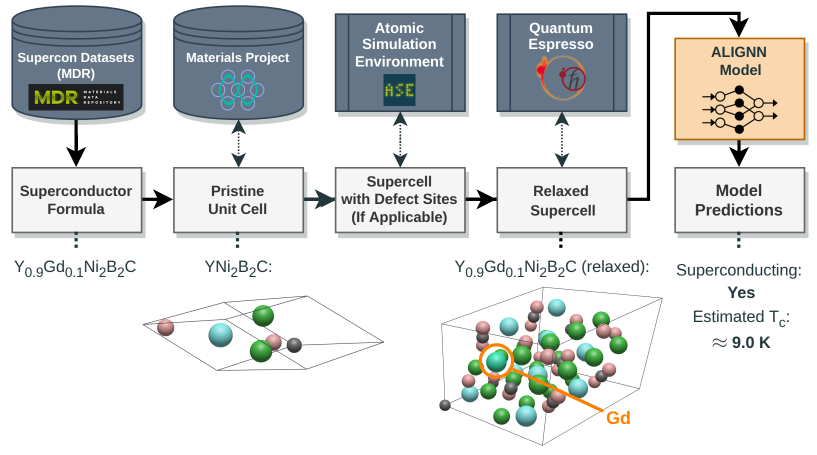




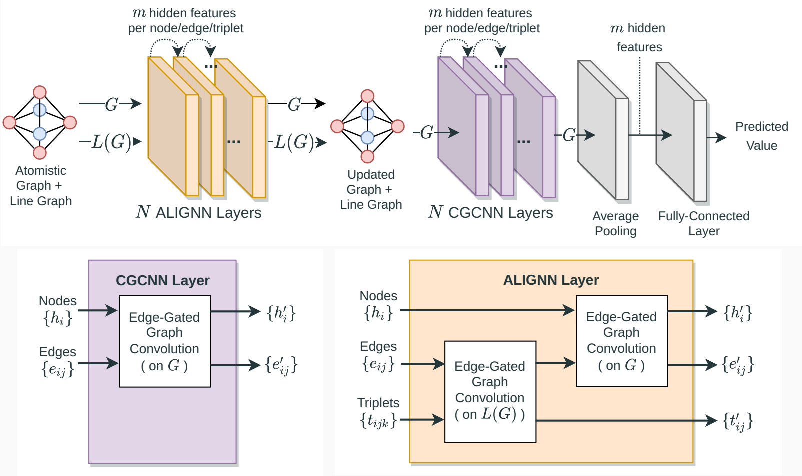
- These datasets had T_c measurements, chemical formulas, and other important metadata, but no atomic structure.

Generating Atomic Structures

Data Generation Pipeline



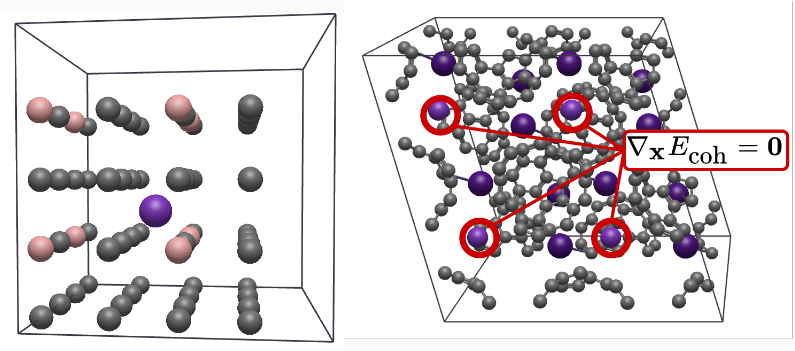
ALIGNN Model Architecture [XG18][CD21]



Data Sources

- A significant challenge was handling the placement of defects (vacancies, interstitials, etc. via the *Embedded Atom Method* [**?**])

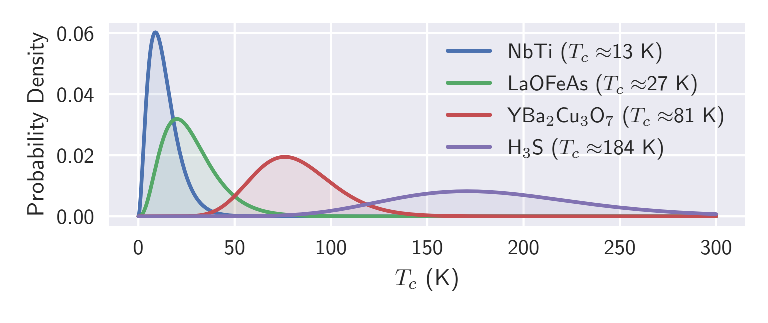
Defect Placement Examples: Fake Lattice (left), KCs_3C_{60} (right).



Experimental T_c Data

- For each superconducting material, many differing measurements were reported due to various factors (applied pressure, choice of substrate, film thickness, etc.)
- We constructed "empirical" distributions of reported T_c values, and had the model predict these distributions:

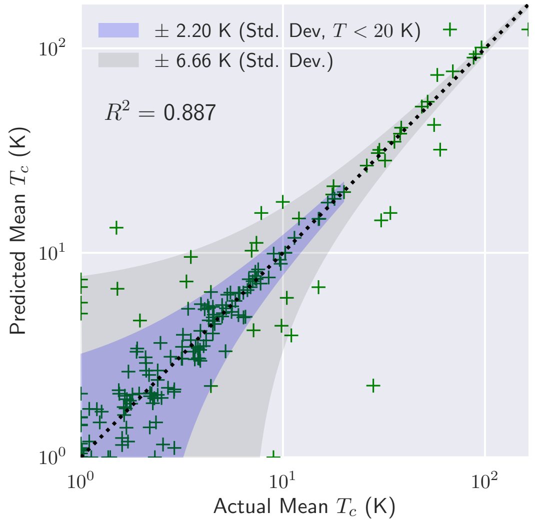
Examples of Empirical T_c Distributions:



Results

Model Evaluation

Predicting Empirical T_c Distributions

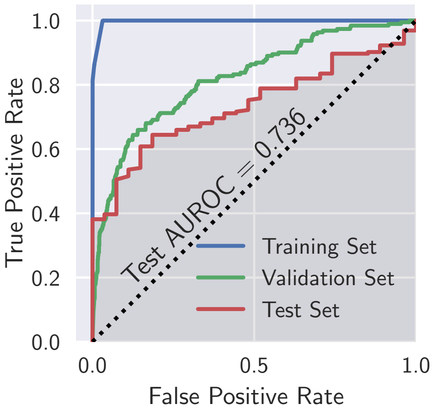


Model Evaluation

Classifying Superconductors (Confusion Matrix and ROC Curve)

		Predicted Superconductor	
		Yes	No
Contained in Dataset	Yes	Total: 102 $TaSe_3$, AlCu, W_2C, Nb_3, RhGe, Ce, $TlNiSe_2$, $SrIr_2$	Total: 92 $LaPd_2Al_3$, Ru_2Zr, In_3Sn, La_3Sn, $PdZr_2$
	No	Total: 95 $YbLuB_{24}$, Ti_3Ir*, $CePb_3$*, $SrAu_5$, $SrGe_3$*	Total: 917 Sc_3Nb, Yb_5Sn_3, $Ba(SmSe_2)_2$, $YAsO_4$, Th_2Zn

*** Materials that are actual superconductors, but were not contained in the dataset.**



Identified Superconductors

- Using the model, we screened over 40,000 metals, oxides, metallic compounds, and hydrides from the Materials Project database [JOH+13].
- We identified over 600 candidate superconductors not contained in our dataset:

Materials Project ID	Formula	Stable	Experimentally Observed	Predicted Mean T_c	Closest Superconductor in Dataset
mp-672238	$CeCuSb_2$	Yes	Yes	1.88 K	Cu_2Sb
mp-1025564	$LuAl_2Pd_5$	Yes	No	8.12 K	Pd
mp-10898	$ScAlNi_2$	Yes	Yes	1.25 K	Ni_3Al
mp-573601	Th_7Ru_3	Yes	Yes	0.95 K	Th
mp-28280	$K_5V_3O_{10}$	Yes	Yes	4.93 K	KO_3
mp-1224184	$HfZrB_4$	Yes	No	2.57 K	HfB_2
mp-1228895	$AlGaSb_2$	No	No	4.15 K	AlSb
mp-1222266	Lu_3S_4	Yes	No	3.63 K	LuS
mp-1079796	Ti_3Pd	Yes	No	4.24 K	Ti
mp-1218331	Sr_3CaSi_8	No	No	1.88 K	$Sr(Si)_2$
mp-1021328	H_4C	Yes	No	50.97 K	H_2
mp-11494	$LuPb_3$	No	Yes	3.80 K	Pb
mp-1226890	Ce_4H_{11}	Yes	No	331.83 K	CeH_9
mp-22266	GdB_6	Yes	Yes	2.22 K	B
mp-1184695	Ho_3Er	No	No	6.22 K	Ho
...	...	...	...	...	...

Conclusion

Conclusion

- We trained a structure-based graph neural network model (ALIGNN) to predict the T_c with a standard deviation error of 6.66 K ($2.20K$ for low-T_c).
- After screening the Materials Project database, we found more than 600 candidate superconductors.

Ongoing and Future Work

- We are currently collaborating with an inorganic chemistry lab at Baylor University to synthesize some of the more promising candidates.
- Additional work needs to be done incorporating electronic features (e.g. band structure) and incorporating structural features (e.g. substrates) into the model.

Questions

Superconductor Candidates List

https://cburdine.github.io/files/qce23.html

GitHub repository: https://github.com/cburdine/sc-screening

For more detailed questions, email: `colin_burdine1@baylor.edu`

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