Non-Classical Methods for the Simulation and Design of Quantum Materials

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Introduction and Motivation

Motivation: Materials Science Perspective

- Materials Science has advanced in various paradigms [AC16].
- Each paradigm is defined by the novel tools and theories developed to understand new physical phenomena:

053208-2 A. Agrawal and A. Choudhary APL Mater. **4**, 053208 (2016)

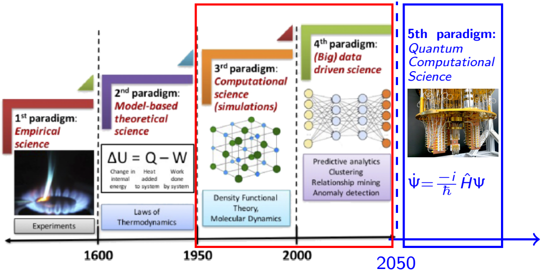
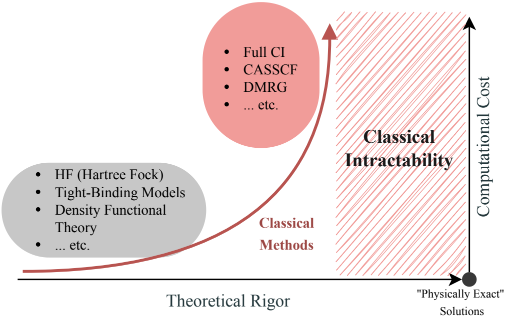


FIG. 1. The four paradigms of science: empirical, theoretical, computational, and data-driven.

- However, due to the failure of classical computational methods to model quantum materials at scale, new tools are required.

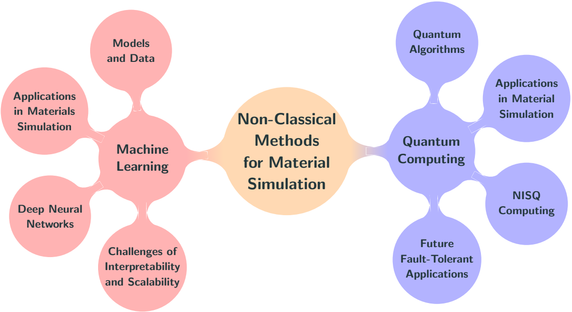
Classical Effective Models

- Finding an exact solution to the electronic ground state is intractable on a classical computer (requires diagonalizing $\hat{H}$).
- One common solution is to find an effective $\hat{H} = \sum_{i,j} h_{ij} \hat{c}_i^\dagger \hat{c}_j$ that approximately accounts for second-order (Coulomb) terms.
- Classical computational methods can accomplish this at various degrees of physical rigor and scale, but they can be quite costly:



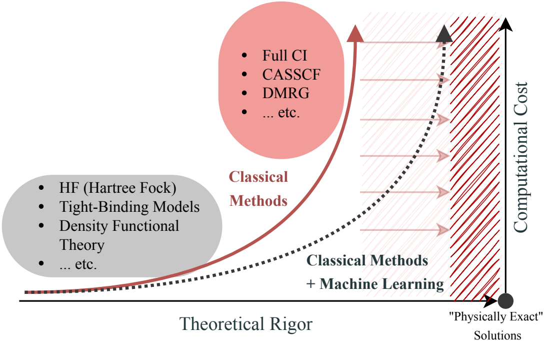
Non-Classical Methods

- My research studies alternatives to classical methods, which I refer to here as non-classical methods.
- Specifically, I focus on how emerging computational techniques and technologies like machine learning and quantum computing can be applied to solve problems beyond the reach of classical methods:



Machine Learning

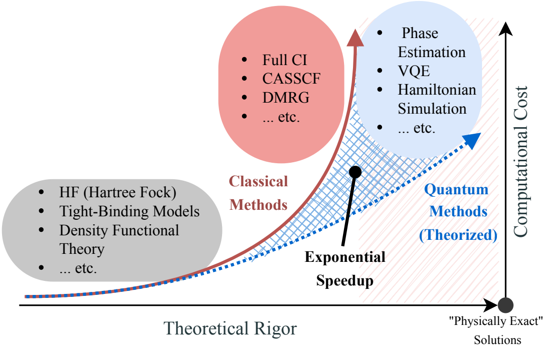
- Augmenting classical methods with machine learning surrogates has shown a strong ability to reduce computational cost.
- This enables new kinds of problems to be solved which were previously considered to be intractable:



- Achieving this speedup requires lots of reliable training data.

Quantum Advantage in Chemistry

- The electronic structure problem can be solved on a quantum computer using Phase Estimation and VQE (Variational Quantum Eigensolver) methods [PM19, BGMT17, ESL+20].
- For Hamiltonians with local interactions, quantum computing methods can give up to an exponential speedup for certain systems [CST+21, DBK+22]:



My Dissertation Research

Overview of Projects

Here, I will focus on three projects, highlighting my recent applications of non-classical methods for materials simulation:

1. High-throughput screening study of superconductors
2. Simulating open quantum systems on quantum computers
3. Quantum-informed neural networks (QuINNs) for electronic structure modeling

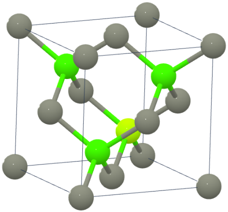
If time, we can also discuss future directions of these projects and and my ongoing work.

High-Throughput Screening of Superconductors with Machine Learning

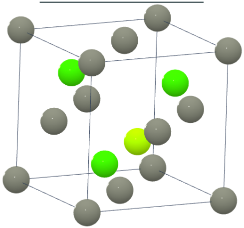
Graph Neural Networks for Material Property Prediction

- Predicting material superconductivity can be viewed as an atomic structure-property learning problem.
- Atomic structures are naturally interpreted as periodic graphs (networks of nodes connected by edges):

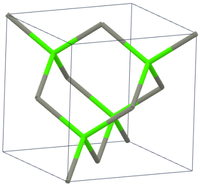
Crystal (graph)



Atoms (nodes)



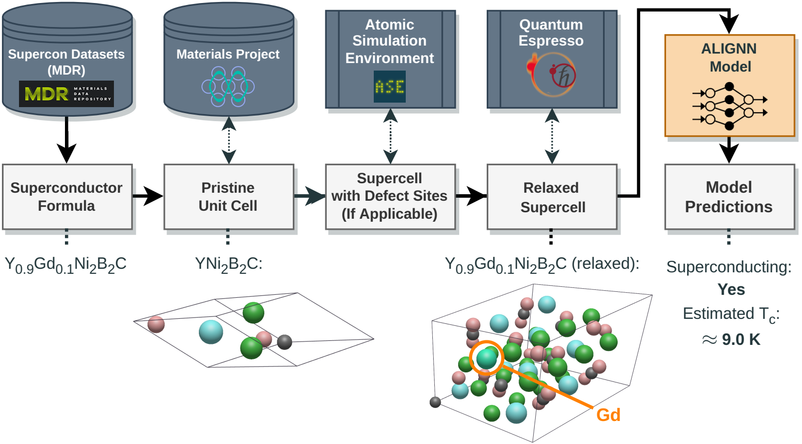
Bonds (edges)



- Graph neural networks are neural network models that make predictions from labeled graphs.
- Crystal structure graphs contain node labels (e.g., atomic species), and edge labels (e.g., bond lengths and bond angles).

Superconductor Dataset Pipeline

Data Generation Pipeline



Identified Superconductors

- We trained ALIGNN to classify superconductors (Acc: $\sim 90\%$, AUROC: 0.74) and estimate T_c (Err: $\pm 2.2K$), and then used the model to screen over 40,000 novel metals, oxides, 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 Known Superconductor
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	V
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
...	...	...	...	...	...

For the complete database of candidate materials visit: https://cburdine.github.io/files/qce23.html

Simulation of Open Quantum Systems on Quantum Computers

Open Quantum Systems

- Understanding the environmental conditions (e.g., high pressure, low temperature, low disorder) that facilitate quantum behavior is crucial to engineering quantum materials [BP02].
- This requires treating a material as an open quantum system.
- We represent open systems by a density matrix $\rho = \sum_{n=1}^{N} p_n \Psi_n \Psi_n^\dagger$. ($n \times n$ for non-interacting electrons, $2^N \times 2^N$ for interacting).
- Open system dynamics are modeled by the Lindblad equation:

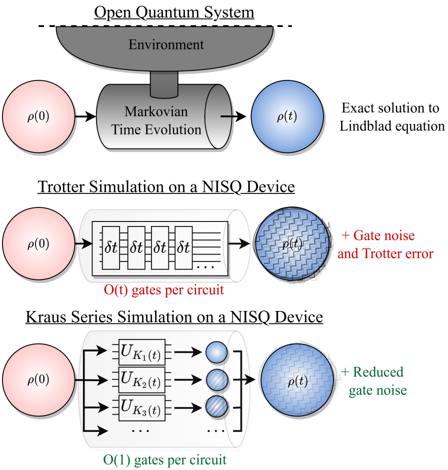
Lindblad Equation

- $\hat{L}_i$: Lindblad operators (environment interaction modes)
- γ_i: Environment coupling coefficients (decay rates)

$$\frac{\partial}{\partial t}\rho = \underbrace{\frac{-i}{\hbar}[\hat{H}, \rho]}_{\text{Schrödinger (reversible)}} + \underbrace{\sum_i \gamma_i \left(\hat{L}_i \rho \hat{L}_i^\dagger - \frac{1}{2}\{\hat{L}_i^\dagger \hat{L}_i, \rho\} \right)}_{\text{Dissipative evolution (non-reversible)}} \quad (1)$$

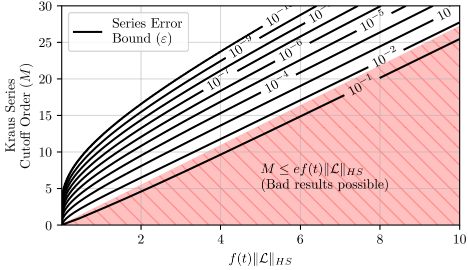
Solving the Lindblad Equation on a Quantum Computer

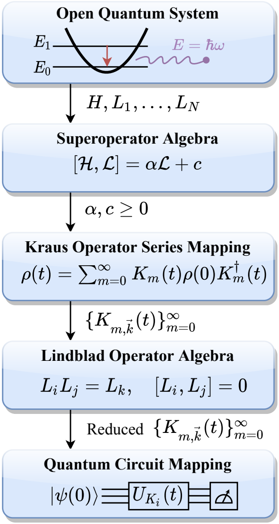
- Existing quantum computing methods employ a numerical time-stepped method called Trotterization. [Tro59]
- This method is not ideal for NISQ devices, because it produces deep circuits.
- We developed a new simulation method that employs Kraus series representations.
- This distributes the computation over many short quantum circuits, reducing device noise.



The Time-Perturbative Kraus Series Method

- Our method expands the evolution of ρ as a time-perturbative Kraus operator series: $\rho(t) = \sum_{m=0}^{\infty} K_m(t)\rho(0)K_m(t)^\dagger$
- Each $K_m(t)$ (up to a cutoff order M) is mapped to a t-parameterized quantum circuit of bounded depth.
- We proved asymptotically linear scaling of M with evolution time t:



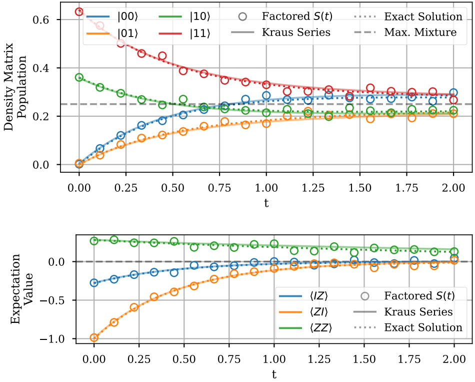


Simulation of Pauli Channels

- A Pauli Channel models decoherence in the qubits on a quantum processor or spin states in magnetic materials.
- For this system, we can even apply all Kraus operators in a superposition $S(t)$, yielding an exponential quantum advantage over naive classical simulation.

Two-qubit Crosstalk Channel

- $H, L_1, L_2, L_3, L_4 = 0, IX, XI, ZZ, XX$
- $\gamma_1, \gamma_2 = 1.0$ (Qubit bit-flip errors)
- $\gamma_3, \gamma_4 = 0.1$ (Cross-talk interactions)



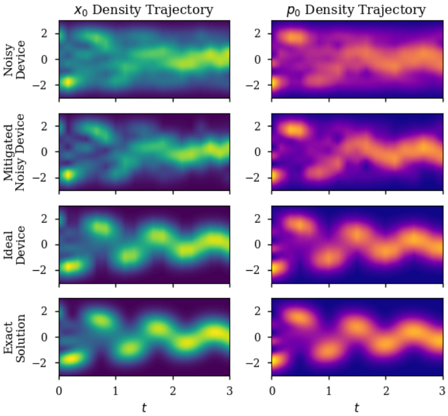
(Results obtained on the Quantinuum H1-1 Quantum Device, July 2024)

Simulation of Bosonic Systems & Harmonic Oscillators

- A single mode containing indistinguishable Bosons with energy $E = \hbar\omega$ can be modeled by a quantum harmonic oscillator.
- We model particle loss by applying a damping operator $L_1 = \hat{a}$ to the oscillator.
- When simulating on NISQ devices, noise must be suppressed through error mitigation.

Damped Harmonic Oscillator

- $H = \hbar\omega(\hat{a}^\dagger a + 1/2) = \hbar\omega(\hat{p}_0^2 + \hat{x}_0^2)/2$
- $L_1 = \hat{a} = (\hat{x}_0 + i\hat{p}_0)/\sqrt{2}, \quad \gamma_1 = 1.0$

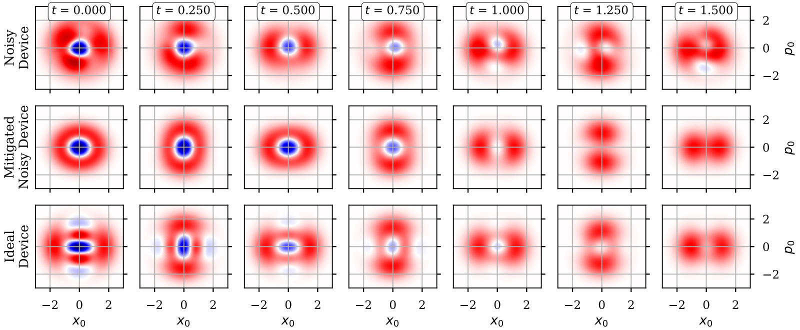


(Results obtained on the IonQ Harmony Quantum Device, June 2024)

Simulating Phase-Space Dynamics

- Quantum Bosonic systems exhibit behavior that is radically different from classical field-mediated interactions.
- This is observed by simulating the Wigner Quasi-probability distribution.

Simulated Wigner Distribution of a "Schrodinger's Cat" State



(Results obtained on the Quantinuum H1-1 Quantum Device, July 2024)

Quantum-Informed Neural Networks for Electronic Structure Modeling

Mean-Field Material Hamiltonians

- Consider an electronic Hamiltonian for periodic material lattices:

$$\hat{H} = \underbrace{\underbrace{\sum_{i,j \in (\text{lattice})}^{N} h_{ij} \hat{c}_i^\dagger \hat{c}_j}_{N \times N \text{ Matrix Representation}} + \sum_{i,j,k,l=1}^{N} v_{ijkl} \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_k \hat{c}_l}_{2^N \times 2^N \text{ Matrix Representation}} \tag{2}$$

(Here $i = (n_i, \vec{r}_i)$, where n_i is an orbital index and $\vec{r}_i$ is a site position)

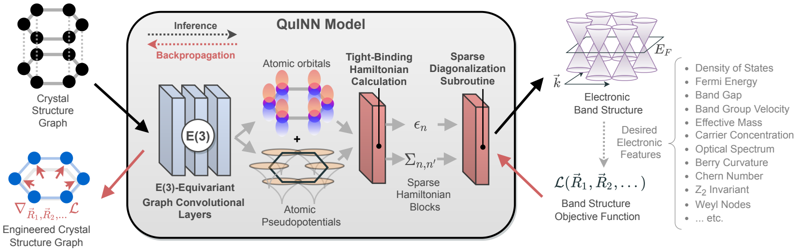
- For electrons that are tightly bound to the lattice sites, we derive an effective mean-field Hamiltonian via the tight-binding approximation:

$$\hat{H}(\vec{k}) = \sum_{i,j \in (cell)} e^{i\vec{k}\cdot(\vec{r}_i - \vec{r}_j)} \tilde{h}_{ij} \hat{c}_i^\dagger \hat{c}_j \tag{3}$$

- Above $\vec{k}$ is a crystal momentum vector in the reciprocal lattice cell.

QuINN: Quantum-Informed Neural Network Models

- To predict electronic band structure, we have developed a new graph neural network architecture (QuINNs):

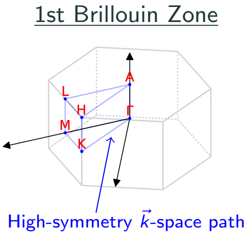


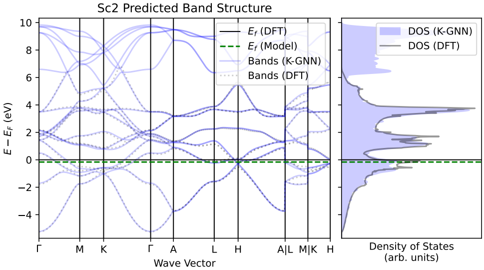
- Since QuINNs are informed by quantum mechanics, they can be used to reverse-engineer effective material Hamiltonians and atomic orbitals from electronic structure data.
- This architecture makes more interpretable predictions than existing models (like ALIGNN), which are not quantum-informed.

Predicting Band Structure and Density of States

- QuINN models allow for high-resolution sampling of $\vec{k}$-space at minimal computational expense (needed for density of states, Fermi surfaces, Green's functions, etc.).
- Computing QuINN bands for each $\vec{k}$-point requires a single sparse diagonalization ($\approx O(N^2)$ via the Lanczos algorithm).
- DFT requires many diagonalization steps, each $O(N^3)$.

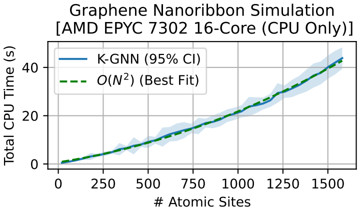
Example: HCP Scandium, K-GNN (QuINN prototype model)

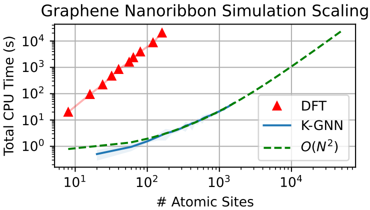




QuINN Model Efficiency

- Basic QuINN models compiled through our QuINN Python package's PyTorch backend have demonstrated $O(N^2)$ scaling.





- Preliminary results suggest that during CPU inference, $10\times$ to $1000\times$ speedups can be achieved over plane wave DFT methods.
- QuINNs also generalize reasonably well to unseen structures:

Dataset	Sc (3D, stable)	Lu (3D, stable)	Dy (3D, stable)	C (2D & 3D, strained)	hBN (2D, strained)
Validation Set Band RMSE	**0.069 eV**	**0.122 eV**	**0.738 eV**	**0.281 eV**	**0.195 eV**

Future and Ongoing Work [Skip]

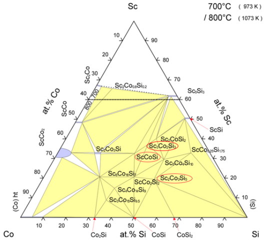
Future and Ongoing Work (Quantum Computing)

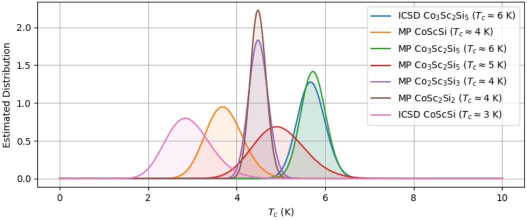
- We have demonstrated that our algorithm allows for accurate simulation of open quantum systems on NISQ hardware.

- Future directions to explore include:
  - Characterizing the kinds of systems where our method yields an exponential quantum advantage.
  - Exploring error mitigation/correction techniques to improve simulation fidelity.
  - Apply Kraus series methods for more efficient subsystem embeddings within VQE (Variational Quantum Eigensolver) methods.

Screening of Superconducting Materials (Ongoing Work

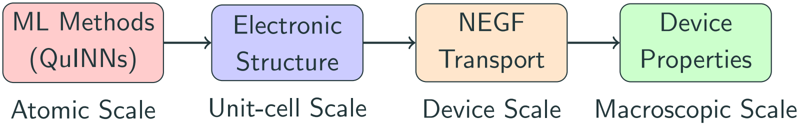
- We have collaborated with Dr. Julia Chan's Lab (Baylor) to attempt synthesis of the most promising intermetallic candidates (Top 10%).
- With further literature review, they confirmed two of the model's top candidate predictions:
  1. La_2Sn_3 (Observed T_c: 2.5 K, Predicted: 2.8 K)
  2. $Lu_3Ir_4Ge_{13}$ (Observed T_c: 2.8 K, Predicted: 1.8 K)
- However, many of the top candidates proved difficult to synthesize:
  - Ce-Bi (oxidizes very rapidly, Exhibits Antiferromag. Kondo Effect)
  - Ce-Te (flammable and toxic, Exhibits Charge Density Waves)
  - Sc-Co-Si (difficulty with synthesis and phase purity)





Future and Ongoing Work (Machine learning)

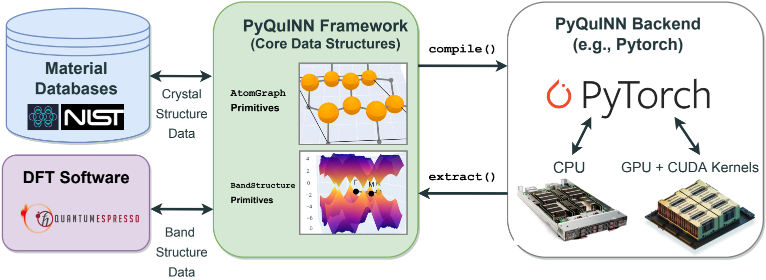
1. **Nanoscale Electronic Device Modeling**
   - QuINNs can be integrated with with Non-Equilibrium Green's Function (NEGF) transport models.
   - NEGF Theory is necessary to bridge atomic-scale and macroscopic-scale electronic simulations of quantum devices:



2. **Hybrid Classical–Quantum Simulation**
   - QuINNs can compress Hamiltonians for resource-efficient quantum algorithms (reduced qubit counts and circuit depth for VQE).
   - The PyQuINN framework can also compute differentiable 2nd-quantized Hamiltonians for hybrid variational optimization.

The PyQuINN Framework

- We have written a framework for QuINN models entirely using Pytorch operations, allowing for efficient CPU inference and GPU training:



- We are working toward packaging and distributing this framework as open-source software on the Python Package Index.
- The PyPI launch is planned for late April, 2026.

Questions

Scan to download these slides:

https://cburdine.github.io/files/lanlintroslides.pdf

For additional questions and feedback, email: `colin_burdine1@baylor.edu`

Acknowledgments

- **Dr. Julia Chan's Lab** (Baylor University)
  - Superconductor Synthesis
- **Nora Bauer** and **Dr. George Siopsis** (University of Tennessee Knoxville)
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- IonQ and Microsoft Azure Quantum
  - Access to Quantum Hardware, Compute Credits
- **Nischal Gautam** (Baylor University)
  - Collaboration on NEGF extensions of PyQuINN.
- **Dr. Enrique P. Blair** (Baylor University)
  - Advisor, Mentor, Collaborator

First-Author Publications

- [BBSB25] **C. Burdine**, N. Bauer , G. Siopsis , E. P. Blair. "Efficient Simulation of Open Quantum Systems on NISQ Trapped-Ion Hardware". In: *Advanced Quantum Technologies* (2025), p. 2400606
- [BB25] **C. Burdine**, E. P. Blair. "Trotterless simulation of open quantum systems for NISQ quantum devices". In: *Advanced Quantum Technologies* 8.1 (2025), p. 2400240
- [BB23] **C. Burdine**, E. P. Blair. "Discovery of novel superconducting materials with deep learning". In: 2023 IEEE International Conference on Quantum Computing and Engineering (QCE). vol. 1. IEEE. 2023, pp. 1335–1341
- [BB26] **C. Burdine**, E. P. Blair. "Quantum-Informed E(3)-Equivariant Neural Networks for Material Design and Quantum Device Engineering". In: (*In Preparation*)

Presentations and Talks

- [Bur25b] **C. Burdine**. "Quantum-Informed Machine Learning for Rapid Material Design and Quantum Device Engineering". In: Texas Quantum Summit (College Station, TX, Sept. 19–21 2025). 2025
- [Bur25a] **C. Burdine**. "Materials + ML". in: 2025 Baylor Materials and Machine Learning Workshop (Waco, TX, June 9–20 2025). 2025
- [Bur24] **C. Burdine**. "Efficient Simulation of Open Quantum Systems on NISQ Quantum Computers". In: Baylor University ECS Research Showcase (Waco, TX, Apr. 26, 2024). 2024
- [Bur23a] **C. Burdine**. "Discovery of novel superconducting materials with deep learning". In: IEEE Interna- tional Conference on Quantum Computing and Engineering (QCE) (Bellevue, WA, Sept. 16–21, 2023). 2023
- [Bur23b] **C. Burdine**. "Predicting the Critical Temperature of Doped and Alloyed Superconductors". In: Southwest Data Science Conference (Waco, TX, Mar. 24, 2023). 2023

Thank you!

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Additional Slides and References

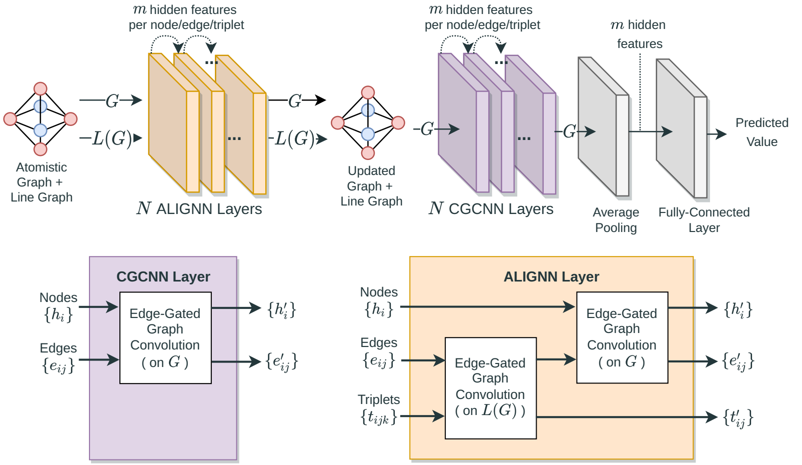
ALIGNN Model Details

ALIGNN Model Summert

- I used the Atomistic Line Graph Neural Network (ALIGNN) model for both classifying superconductors and predicting T_c [CD21].
- ALIGNN is one of the top performing deep learning models for structure-based material property predictions. [DWG$^+$20].
- Pros:
  - Is naturally invariant under $E(3)$ (Euclidean) symmetries and space group symmetries.
  - Time complexity is $\mathcal{O}(n)$ (by comparison DFT is $\mathcal{O}(n^3)$).
  - Incorporates both bond lengths and bond angles.
- Cons:
  - Bond features are not quantum-informed; Lacks interpretability.
  - Prone to overfitting and requires lots of data to perform well.
  - Cannot distinguish the chirality of structures (not fully equivariant).

ALIGNN Model

ALIGNN Model Architecture [XG18][CD21]



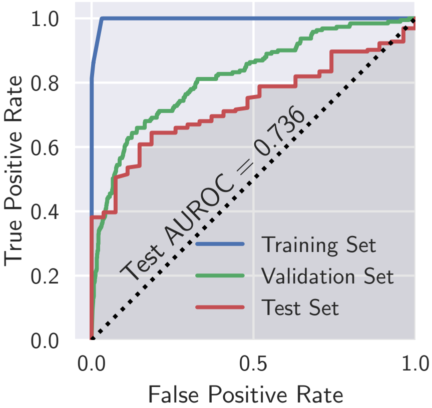
Superconductor Model Evaluation

Model Evaluation

Classifying Superconductors (Confusion Matrix and ROC Curve)

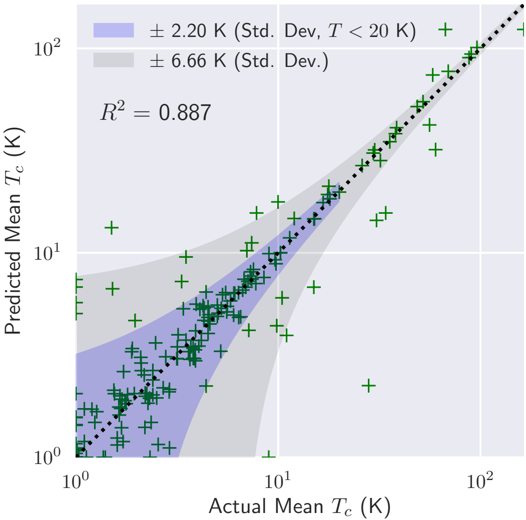
		Predicted Superconductor: Yes	Predicted Superconductor: No
Contained in Dataset	Yes	**Total: 102** $TaSe_3$, AlCu, W_2C, Nb_3, RhGe, Ce, $TlNiSe_2$, $SrIr_2$	**Total: 92** $LaPd_2Al_3$, Ru_2Zr, In_3Sn, La_3Sn, $PdZr_2$
Contained in Dataset	No	**Total: 95** $YbLuB_{24}$, Ti_3Ir*, $CePb_3$*, $SrAu_5$, $SrGe_3$*	**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.



Model Evaluation

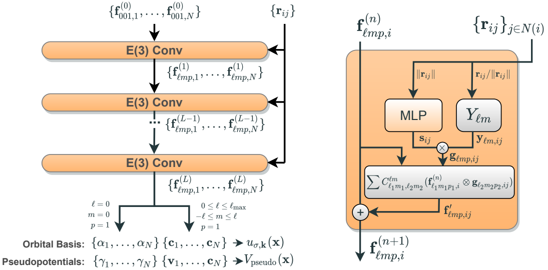
Predicting Empirical T_c Distributions



More About QuINNs

E(3) Equivariant Graph Neural Networks

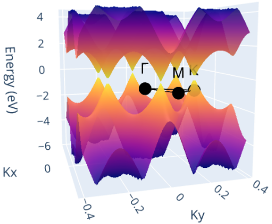
- To predict the orbital and pseudopotential parameters we employ E(3)-equivariant graph neural network layers.
- These layers respect all crystal translation, rotation, and reflection symmetries in E(3) (the Euclidean group) and parameterize the Gaussian orbital & potential coefficients α_i, c_i and γ_i, v_i:

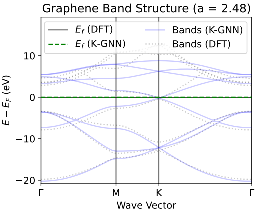


- $E(3)$ graph convolutions are performed in terms of spherical harmonic coefficients $\mathbf{f}_{\ell mp}$ (called irreducible representations).

Example: QuINN Carbon Allotropes Model

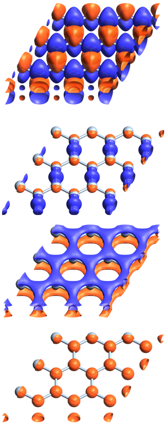
- We first trained a QuINN model on a small dataset of graphene atomic structures.
- Graphene is a 2D material consisting of C atoms bound in a honeycomb lattice.





- The model predicts the clear presence of Dirac cones at the $\vec{k} = K$ points.
- The delocalized p_z orbitals forming these cones are responsible for graphene's high carrier mobility and exceptional conductivity properties.

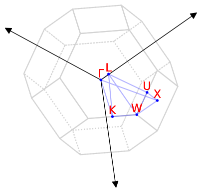
QuINN Γ-point Bloch Orbitals:

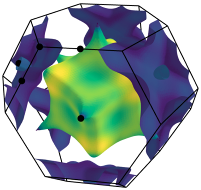


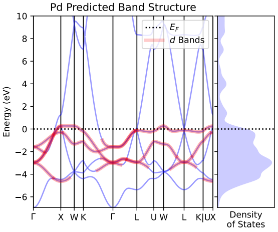
Fermi Surfaces

- An important feature of conducting or semiconducting materials is the topology of the bands that intersect the Fermi energy E_F.
- These band isosurfaces at E_F comprise the Fermi Surface and play an important role in the chemical and topological properties of materials.
- QuINNs allow for rapid high-resolution computation of Fermi surfaces, which is computationally expensive with DFT.

Example: FCC Palladium Fermi Surface

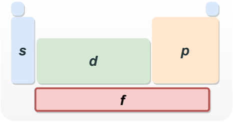




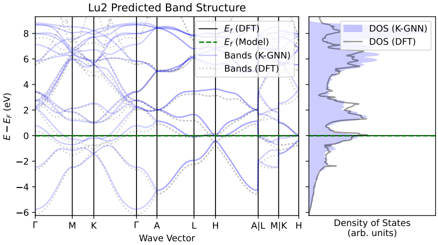


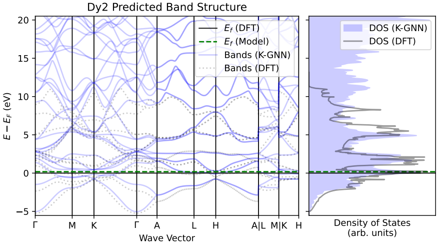
Limitations of QuINNs

- QuINNs can predict valence band structure for all elements of the periodic table, attaining reasonable accuracy on f-block metals, like Lu and Dy.



- However, QuINNs have limited capacity to capture conducting states accurately for heavy atoms.

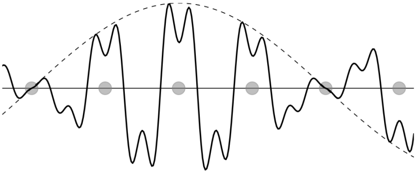


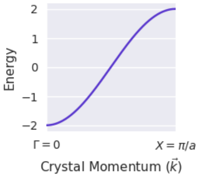


Calculation of Tight-Binding Hamiltonians

Tight Binding Models

- According to Bloch's Theorem, a wave function $\Psi(\vec{x})$ for a periodic crystal satisfies $\Psi(\vec{x}) = e^{i\vec{k}\cdot\vec{r}}\Psi(\vec{x}-\vec{r})$, where $\vec{k}$ is a crystal momentum vector and $\vec{r}$ is a translation vector.





- $\hat{H}$ can then be written as a periodic function of the momentum $\vec{k}$:

$$\hat{H}(\vec{k}) = \sum_{i,j\in(cell)} e^{i\vec{k}\cdot(\vec{r}_i-\vec{r}_j)}\tilde{h}_{ij}\hat{c}_i^\dagger\hat{c}_j \qquad (4)$$

- $H(\vec{k})$ has a continuum of allowed energies (the band structure)

Representing Atomic Orbitals

- The effective Hamitonian coefficients $\tilde{h}_{ij}$ can be approximated as

$$\tilde{h}_{ij} = \langle \phi_i | \, H \, | \phi_j \rangle = \int \phi^*_{n_i}(\vec{x} - \vec{r_i}) H \phi_{n_j}(\vec{x} - \vec{r_j}) d\vec{x} \tag{5}$$

- The integral (5) cannot be evaluated in closed form for Hydrogen-like orbitals $\phi_{n_i}(r, \theta, \varphi)$ and potentials $V(r) \propto 1/r$.
- We use orbitals $\phi(r, \theta, \varphi) = F(r) X'_{\ell,c}(r, \theta, \varphi)$, where $X'_{\ell,c}$ are the (real-valued) solid harmonics:

$$X'_{\ell,c}(r, \theta, \varphi) = i^{n_c} \sqrt{\frac{2\pi}{2\ell + 1}} r^\ell \left[Y_{\ell,m}(\theta, \varphi) \pm Y_{\ell,-m}(\theta, \varphi) \right] \tag{6}$$

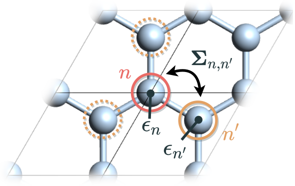
(Above, we use $c = \ell + m$, where $\pm$ denotes sign(m) and $n_c \in \{0, 1, 2, 3\}$)

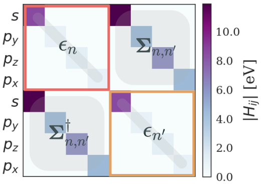
- We also expand $F(r)$ and $V(r)$ as sums of primitive Gaussians:

$$F(r), V(r) \propto \sum_{s=1}^{N_s} c_s e^{-\alpha_s r^2} \tag{7}$$

Gaussian Orbitals and the Tight-Binding Hamiltonian

- We can expand the orbitals and potentials as sums of Gaussian functions times real solid harmonics (this allows the coefficients $\tilde{h}_{ij}$ to be computed in a closed differentiable form).
- From the $\tilde{h}_{ij}$ coefficients, we construct a block-matrix $\mathbf{H}(\vec{k})$ of on-site energies ϵ_n and neighboring site tunneling energies $\Sigma_{n,n'}$:





- The matrix $\mathbf{H}(\vec{k})$ can be diagonalized for each $\vec{k}$ to obtain eigenvalues (band structure) and eigenvectors (Bloch orbitals).

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