

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

Colin M. Burdine

PhD Candidate

February 12, 2026

Baylor University

Department of Electrical and Computer Engineering



Table of contents

1. Introduction: Materials Science Perspectives
2. Motivation and Background
3. My Work in Computational Materials Science
4. Additional Slides and References

Introduction: Materials Science Perspectives

Materials Science

- Materials science is the backbone of technological progress. From ancient tools to modern electronics, each breakthrough has ignited new industries, economies, and ways of living.



- Today, we are entering the age of **quantum materials**, which exhibit effects such as magnetism, superconductivity, and topological or strongly-correlated electronic states.
- These phenomena can be harnessed to develop novel technologies for **sustainable energy**, health, sensing, and information processing.

History of Materials Science

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

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A. Agrawal and A. Choudhary

APL Mater. 4, 053208 (2016)

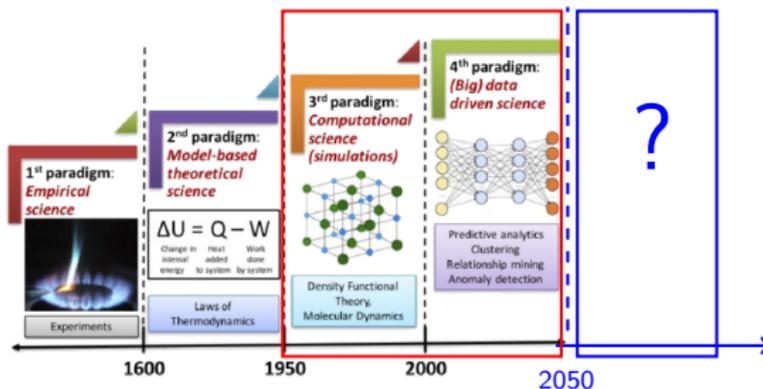


FIG. 1. The four paradigms of science: empirical, theoretical, computational, and data-driven.

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

Motivation and Background

Electronic Structure

- An important problem in chemistry is finding the ground state electronic structure of a crystal or molecule.
- This requires solving the Schrödinger equation with an electronic many-particle Hamiltonian \hat{H} to obtain a system's "allowed" energies E_n .

Electronic Many-Particle Hamiltonian (N modes)

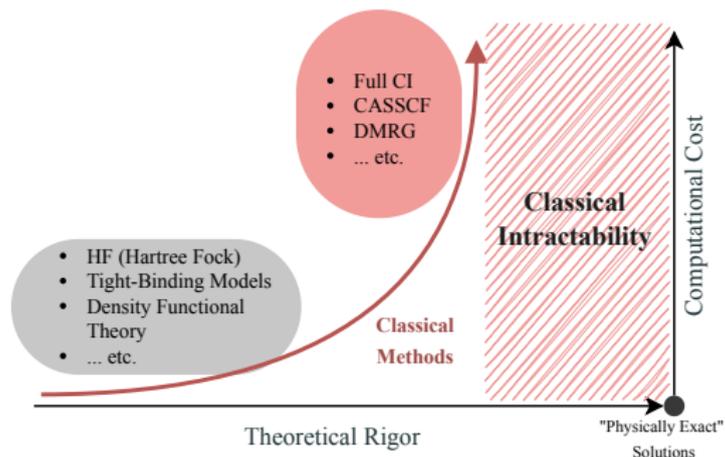
- h_{ij} : on-site and kinetic energies, v_{ijkl} : Coulomb and interaction energies.
- $\hat{c}_i^\dagger/\hat{c}_i$: creation/annihilation operators for an electron in mode i .

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

$2^N \times 2^N$ Matrix Representation

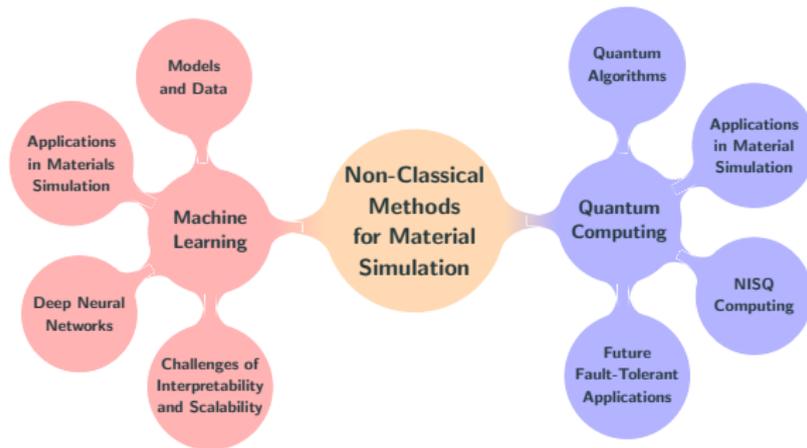
Classical Effective Models

- 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 the intractable v_{ijkl} terms.
- Classical computational methods can accomplish this at various degrees of physical rigor and scale, **but they can be quite costly**:



Non-Classical Methods

- In this presentation, we consider alternatives to classical methods, which we refer to here as **non-classical methods**.
- Specifically, we 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:

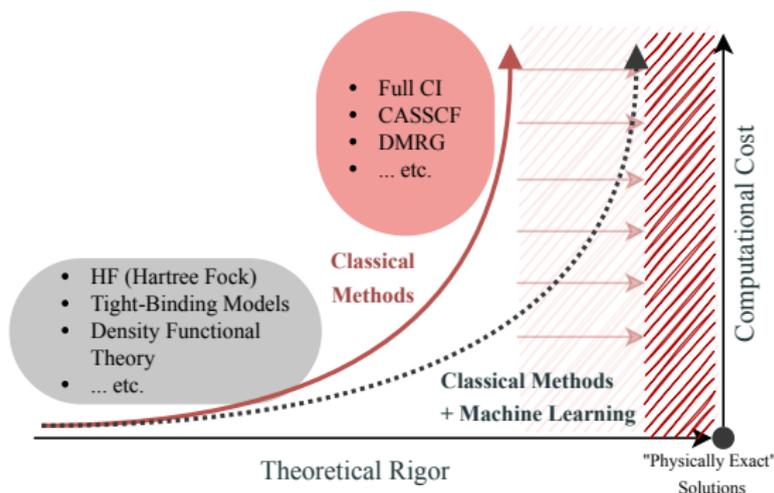


Machine Learning of Electronic Structure

- There is recent interest in applying machine learning to handle the intractability of the electronic structure problem:
 - Learning to identify quantum phase transitions in quantum matter [Car20]
 - Searching for Hamiltonians with topological properties [PSM21]
 - Learning the electron density exchange-correlation functional in DFT [DFS20]
 - Learning interatomic potentials and force fields [GSDV17, KVGC⁺23, BBCR17]
- Neural networks are often used as a surrogate for subroutines that are computationally expensive in order to accelerate existing classical methods.
- Neural networks can also be trained to incorporate the physics of solutions to the Schrödinger equation.
 - We refer to these as **Quantum-Informed Neural Networks (QuINNs)**.

Quantum-Informed Neural Networks

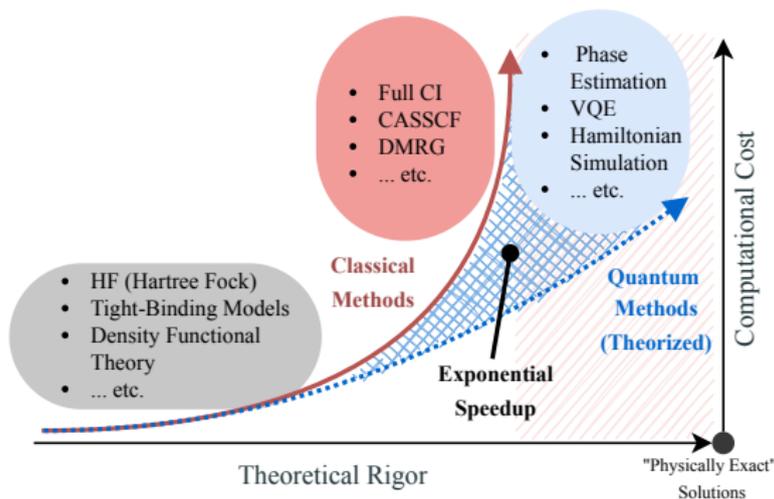
- Augmenting classical methods with machine learning surrogates has shown a strong ability to reduce computational cost.
- This enables new kinds of problems to be solved which were previously considered to be intractable:



- 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 Work in Computational Materials Science

Overview of Projects

In this presentation, 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. Quantum-Informed Neural Networks for Electronic Structure
3. Simulating Open Quantum Systems on Quantum Computers
(At the end, if time permits)

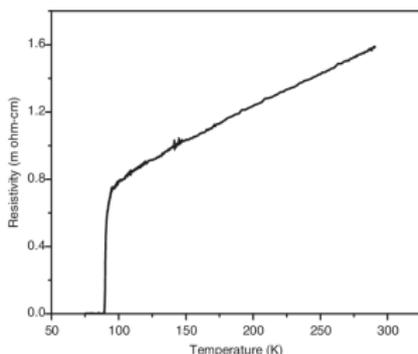
We will also discuss future directions of these projects and how they align with the research goals of SRNL's Hydrogen Isotope Science Team.

Project 1: High-Throughput Screening of Superconductors

Superconductors

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

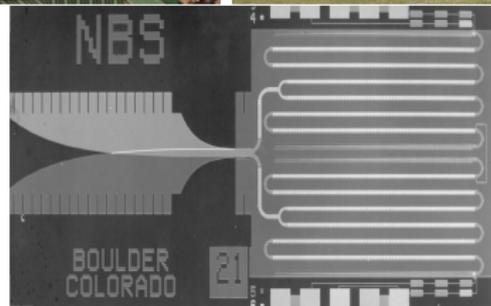
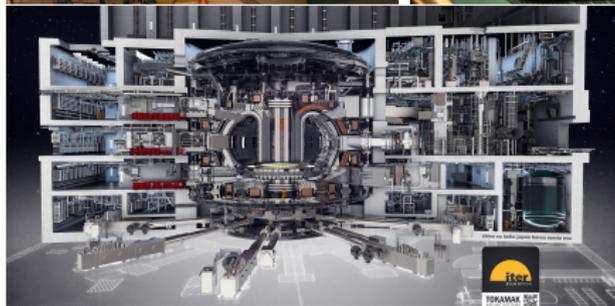
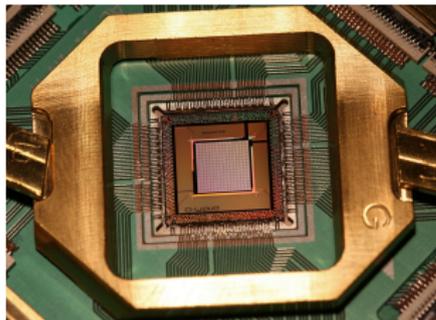
Example: $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ [VBR14]



- A superconductor's **critical temperature** (T_c) is the highest temperature at which it exhibits these two properties.
- Computational *ab initio* modeling is feasible for conventional (BCS) superconductors; **but not for unconventional superconductors.**

Superconductors

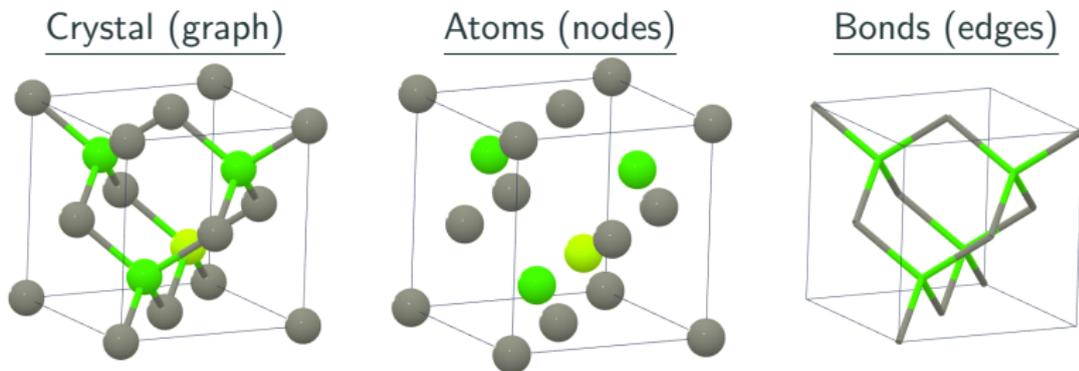
Industrial Applications of Superconductors



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Deep Graph Neural Networks

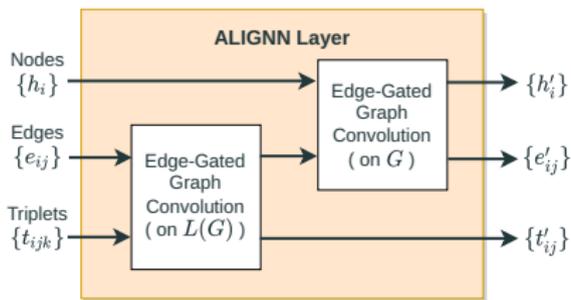
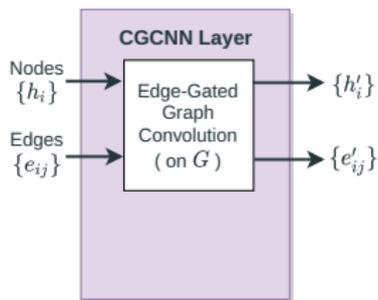
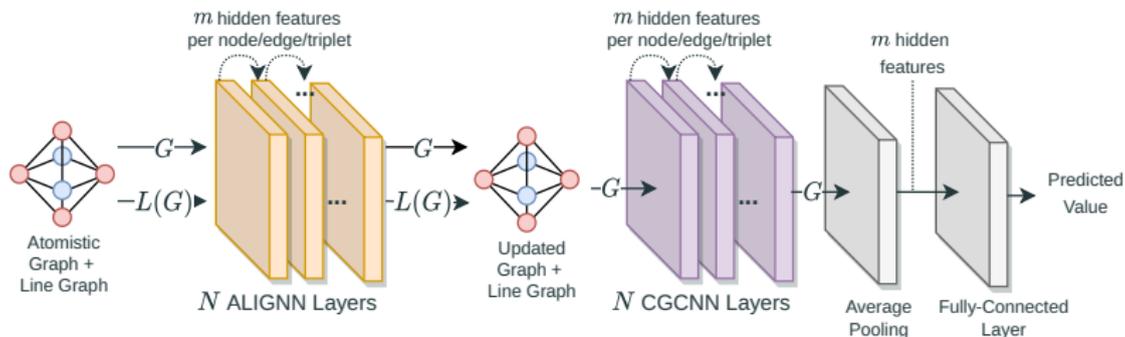
- Predicting superconductivity can be viewed as a structure-property learning problem.
- The ALIGNN model is a **graph neural network** that makes predictions from graphs (networks of nodes and edges).
- Atomic structures are naturally interpreted as periodic graphs:



- In this study we trained and fine-tuned the ALIGNN model to identify superconductors and estimate their T_c **using experimental data** scraped from academic papers.

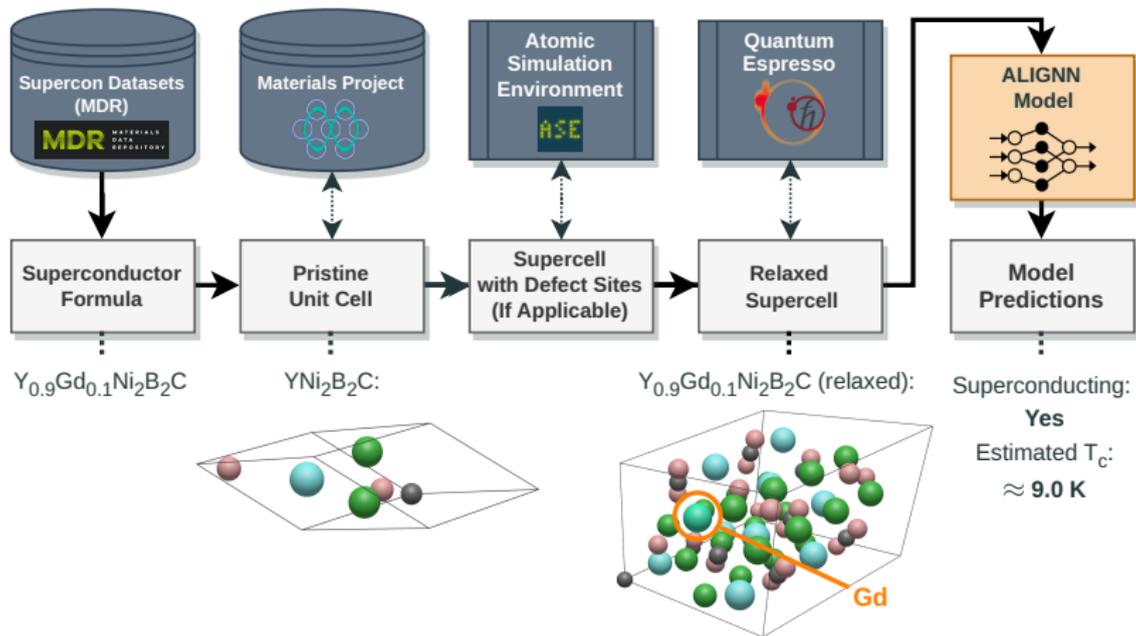
ALIGNN Model

ALIGNN Model Architecture [XG18][CD21]



Generating Superconductor Atomic Structures

Data Generation Pipeline

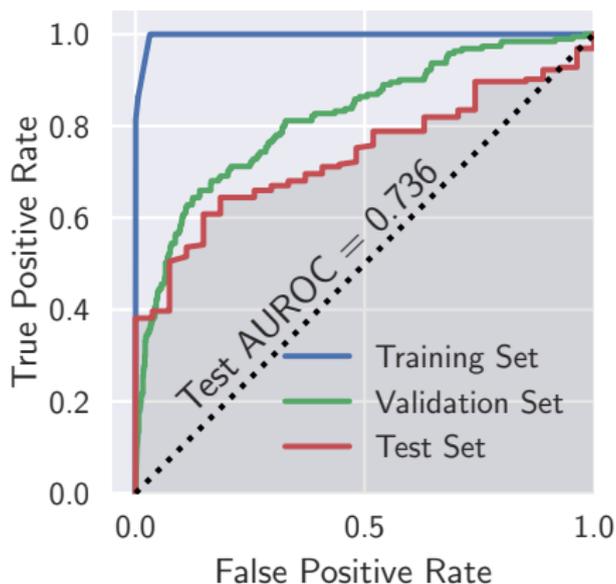


Model Evaluation

Classifying Superconductors (Confusion Matrix and ROC Curve)

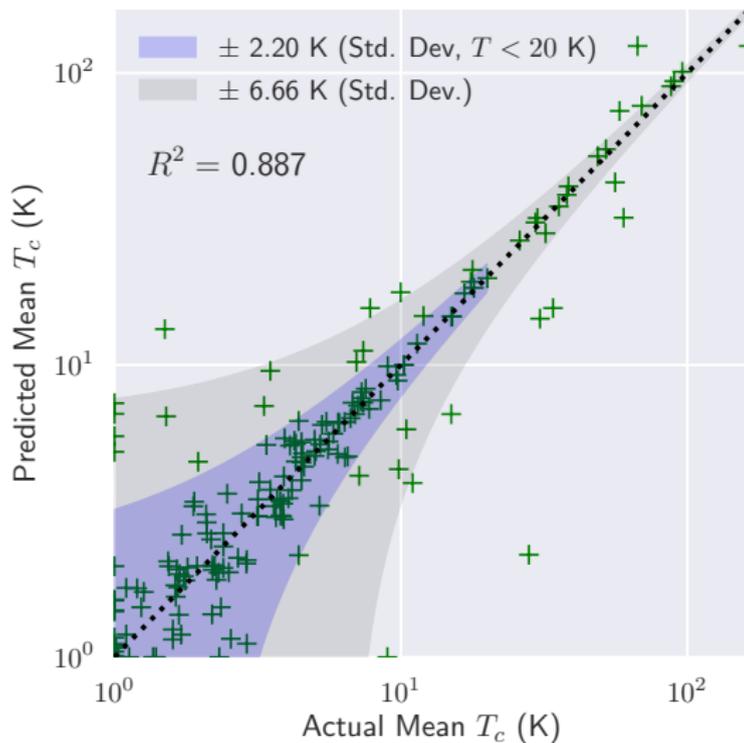
		Predicted Superconductor	
		Yes	No
Contained in Dataset	Yes	<u>Total: 102</u> TaSe ₃ , AlCu, W ₂ C, Nb ₃ , RhGe, Ce, TiNiSe ₂ , Srlr ₂	<u>Total: 92</u> LaPd ₂ Al ₃ , Ru ₂ Zr, In ₃ Sn, La ₃ Sn, PdZr ₂
	No	<u>Total: 95</u> YbLuB ₂₄ , Ti ₃ Ir*, CePb ₃ *, SrAu ₅ , SrGe ₃ *	<u>Total: 917</u> Sc ₃ Nb, Yb ₅ Sn ₃ , Ba(SmSe ₂) ₂ , YAsO ₄ , Th ₂ Zn

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



Model Evaluation

Predicting Empirical T_c Distributions



Identified Superconductors

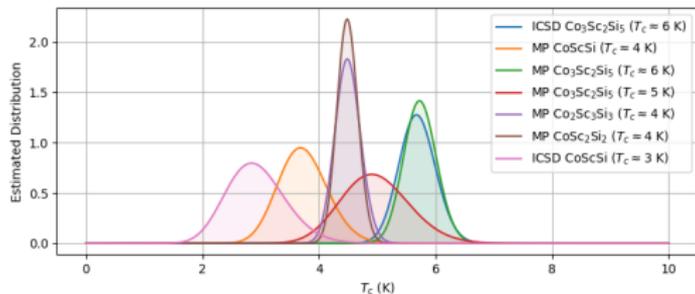
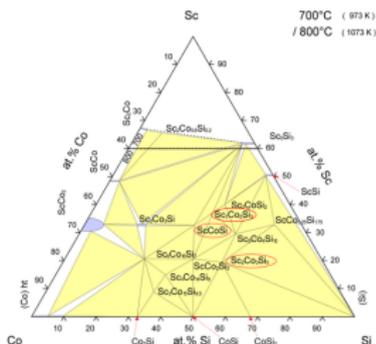
- Using the model, we screened over 40,000 metals, oxides, metallic compounds, and hydrides from the Materials Project database [JOH⁺13].
- We identified **over 600 candidate superconductors** not contained in our dataset:

Materials Project ID	Formula	Stable	Experimentally Observed	Predicted Mean T_c	Closest Known Superconductor
mp-672238	CeCuSb ₂	Yes	Yes	1.88 K	Cu ₂ Sb
mp-1025564	LuAl ₂ Pd ₅	Yes	No	8.12 K	Pd
mp-10898	ScAlNi ₂	Yes	Yes	1.25 K	Ni ₃ Al
mp-573601	Th ₇ Ru ₃	Yes	Yes	0.95 K	Th
mp-28280	K ₅ V ₃ O 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 ₃ S ₄	Yes	No	3.63 K	LuS
mp-1079796	Ti ₃ Pd	Yes	No	4.24 K	Ti
mp-1218331	Sr ₃ CaSi ₈	No	No	1.88 K	Sr(Si) ₂
mp-1021328	H ₄ C	Yes	No	50.97 K	H ₂
mp-11494	LuPb ₃	No	Yes	3.80 K	Pb
mp-1226890	Ce ₄ H ₁₁	Yes	No	331.83 K	CeHg
mp-22266	GdB ₆	Yes	Yes	2.22 K	B
mp-1184695	Ho ₃ Er	No	No	6.22 K	Ho
...

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

High-Throughput Screening of Superconducting Materials

- We 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. $\text{Lu}_3\text{Ir}_4\text{Ge}_{13}$ (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)



Project 2: Quantum-Informed Neural Networks for Electronic Structure Prediction

Tight-Binding Models for materials

- Consider an electronic Hamiltonian for periodic material lattices:

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

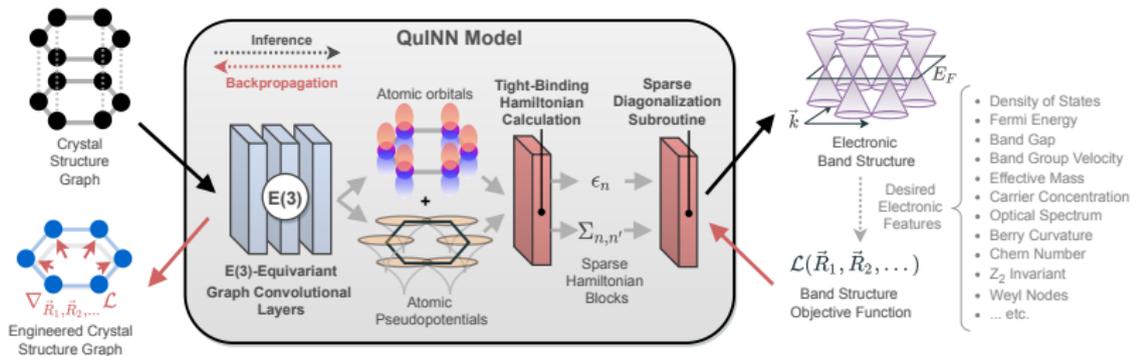
(Here $i = (n_i, \vec{r}_i)$, where n_i is an orbital index and \vec{r}_i is a site position)

- For electrons that are tightly bound to the lattice sites, we derive an effective mean-field Hamiltonian (function of **crystal momentum** \vec{k}):

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

QuINN: Quantum-Informed Neural Network Models

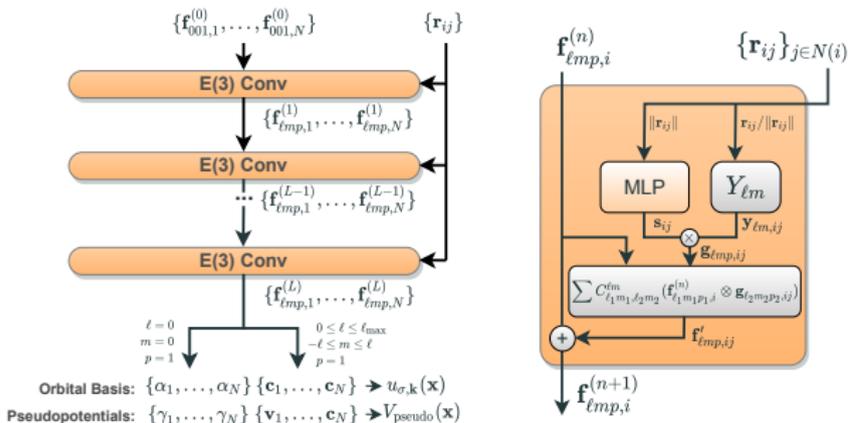
- To predict electronic band structure, we have developed a new graph neural network architecture (QuINNs):



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

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 in 3 dimensions).

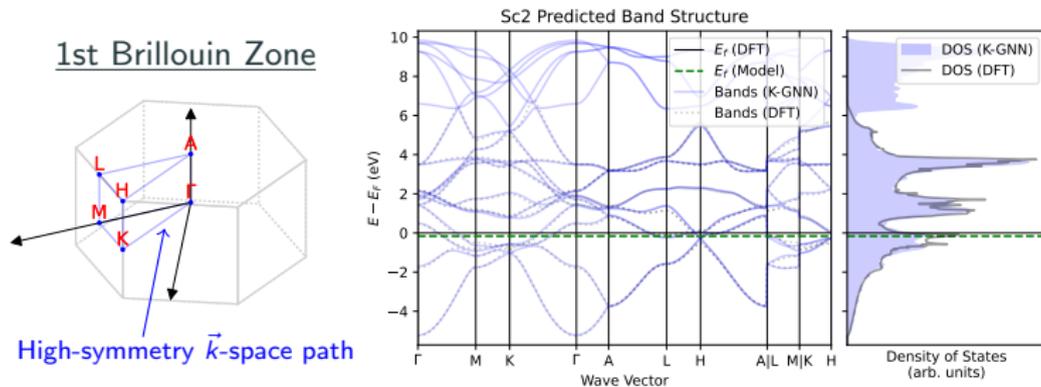


- E(3)** graph convolutions are performed in terms of spherical harmonic coefficients $f_{\ell mp}$ (called **irreducible representations**).

Band Structure and Density of States with K-GNN

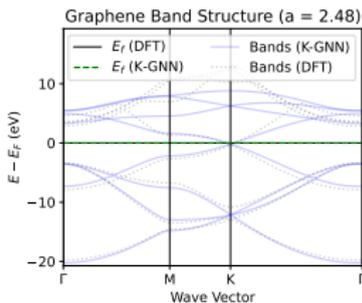
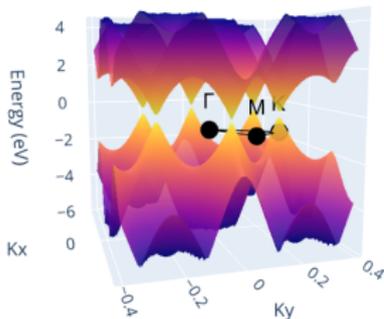
- QuINN models allow for high-resolution sampling of \vec{k} -space at minimal computational expense (needed for density of states, Fermi surfaces, Green's functions, etc.).
- Computing QuINN bands for each \vec{k} -point requires a single sparse diagonalization ($\approx O(N^2)$ via the Lanczos algorithm).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

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



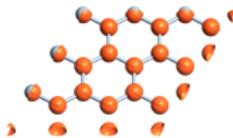
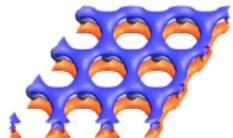
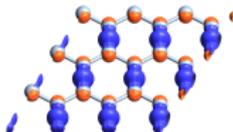
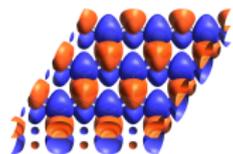
Example: QuINN Graphene Prototype

- 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.



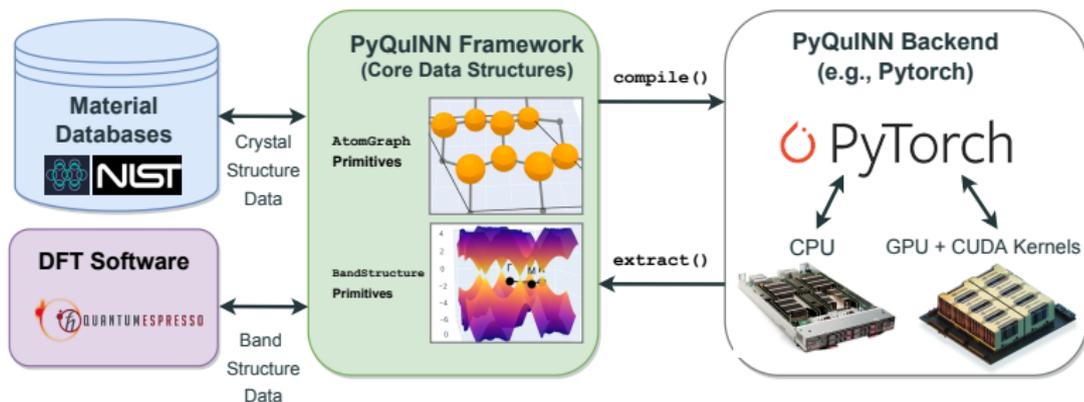
- The model predicts the clear presence of Dirac cones at the $\vec{k} = K$ points.
- The delocalized p_z orbitals forming these cones are responsible for graphene's high carrier mobility and exceptional conductivity properties.

QuINN Γ -point
Bloch Orbitals:



The PyQuINN Framework

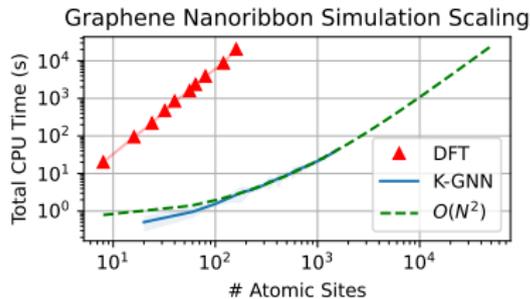
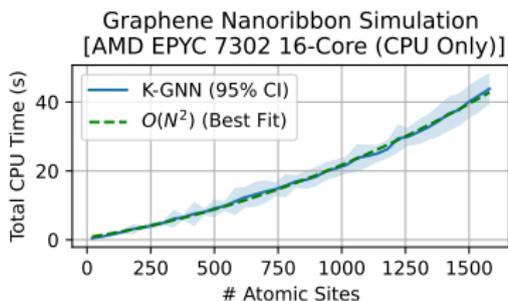
- We have written a framework for QuINN models entirely using Pytorch operations, allowing for efficient CPU inference and GPU training:



- We are working toward packaging and distributing this framework as open-source software (on the Python Package Index).

PyQuINN Model Efficiency

- Basic QuINN models compiled through PyQUINN'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:

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

Connections to SRNL's Research

- Work is currently underway integrating Non-Equilibrium Green's Function (NEGF) methods into PyQuINN.
- NEGF serves as a bridge between quantum-scale modeling and device-scale modeling, enabling accurate modeling of surface chemistry, quantum transport, heat transport, and catalysis.
- This connects to SRNL's recent efforts in novel methods for hydrogen isotope separation via graphene oxide (GO), carbon nanotubes, and quantum molecular sieves.
- QuINNs + NEGF formalisms could enable large-scale molecular dynamics simulation of hydrogen isotope separation devices like GO, with quantum electronic accuracy.
- Integrating QuINNs with ab-initio and heat/phonon transport models could allow for the design of highly resilient materials for extreme conditions (e.g., radiation absorption, heat exchange).

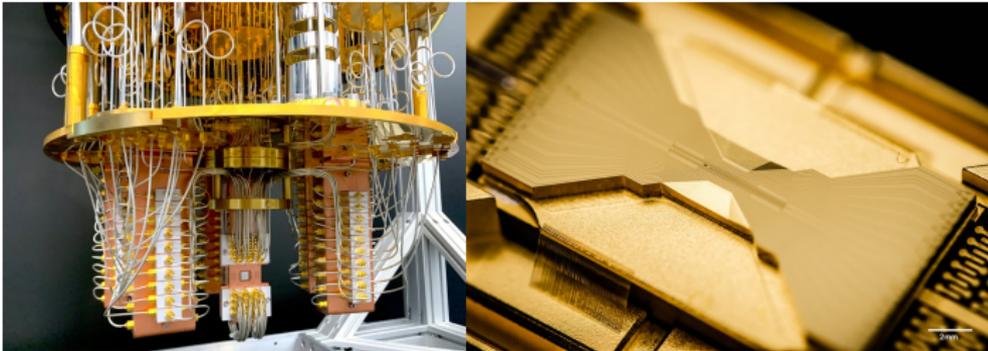
SRNL's Hydrogen Isotope and Fusion Materials Mission

- This research has equipped me with multi-domain computational skills that can be immediately applied in the next 1-2 years to support SRNL's missions:
 1. **Electronic structure and ML modeling** for predicting adsorption energies, diffusion barriers, and isotope selectivity
 2. **QuINNs + DFT + ML** screening for candidate membranes, catalysts, and high-performance alloys via atomistic modeling
 3. **NEGF + Quantum transport modeling** of permeation, surface reactions, and transport in graphene oxides and other 2D materials
 4. **High-throughput computational workflows** for fuel cycle optimization
 5. Versatile **open-source tools for multiscale materials research** (integrating PyQuINN with SRNL HPC infrastructure)

My Research in Quantum Computing **[Skip]**

Overview of Quantum Computing

- Quantum Computing is a new paradigm of computing in which information is represented in **qubits (quantum bits)**.
- Qubits represent a superposition of correlated 0's and 1's, which can be manipulated through operations called **quantum gates**.



- Modern quantum computer processors are called **Noisy Intermediate-Scale Quantum (NISQ)** or **Early Fault-Tolerant** devices.

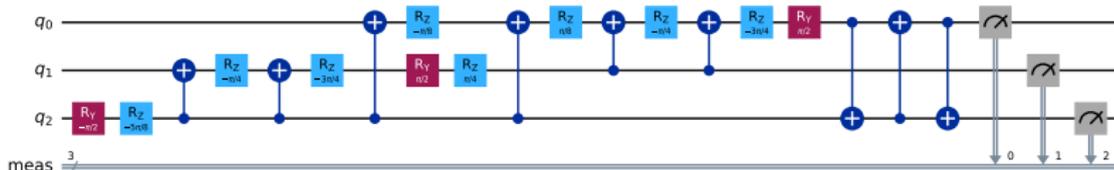
<https://www.popsci.com/technology/in-photos-journey-to-the-center-of-a-quantum-computer/>

<https://arstechnica.com/science/2020/10/trapped-ion-quantum-computer-sets-new-mark-for-quantum-volume/>

Quantum Circuits

- Many qubits together can represent a **wave function** Ψ , which can be manipulated via the principles of superposition and entanglement.
- The final wave function Ψ can then be measured, producing a single sample from the distribution $|\Psi|^2$.
- The process of manipulating a wave function and measuring it can be represented as a **quantum circuit**.

Example: Fourier Transform Quantum Circuit



Project 3: Simulating 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:

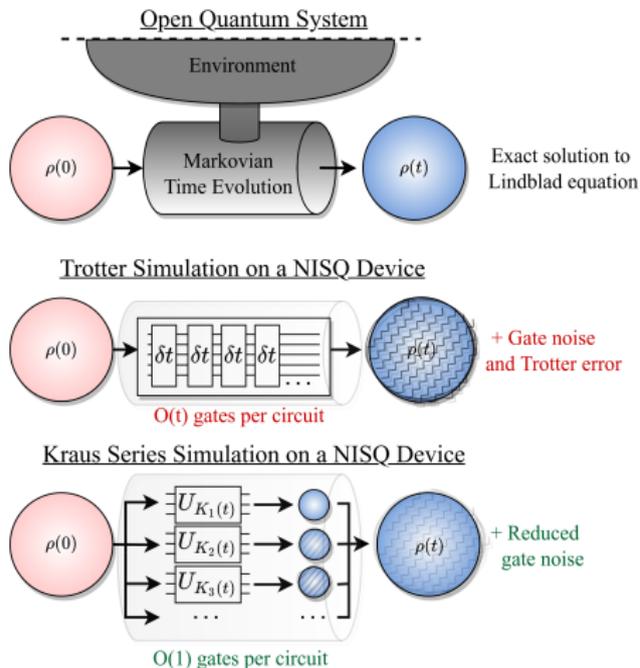
Lindblad Equation

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

$$\frac{\partial}{\partial t} \rho = \underbrace{\frac{-i}{\hbar} [\hat{H}, \rho]}_{\text{Schrödinger (reversible)}} + \underbrace{\sum_i \gamma_i \left(\hat{L}_i \rho \hat{L}_i^\dagger - \frac{1}{2} \{ \hat{L}_i^\dagger \hat{L}_i, \rho \} \right)}_{\text{Dissipative evolution (non-reversible)}} \quad (4)$$

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.

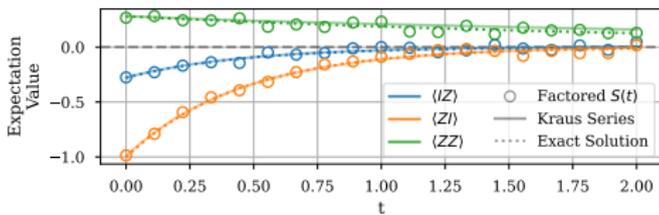
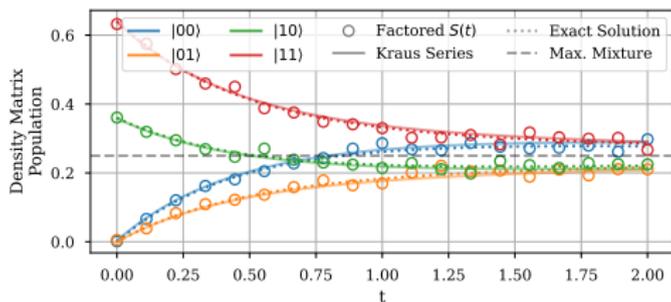


Simulation of Pauli Channels

- 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 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)

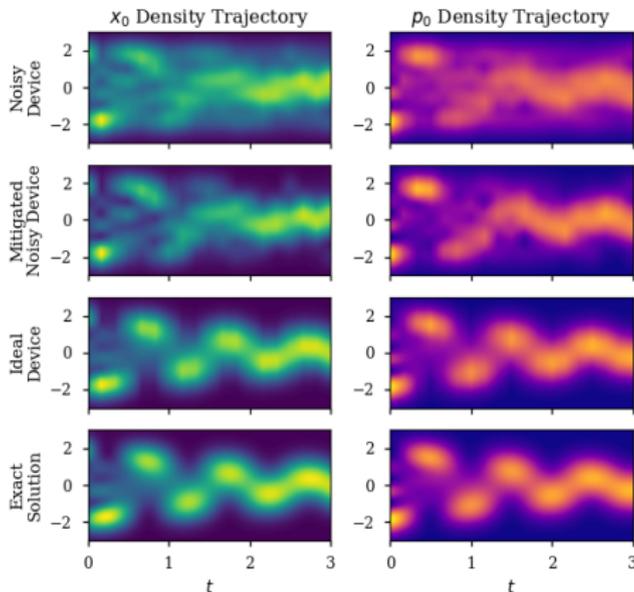


Simulation of Bosonic Systems & Harmonic Oscillators

- 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

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

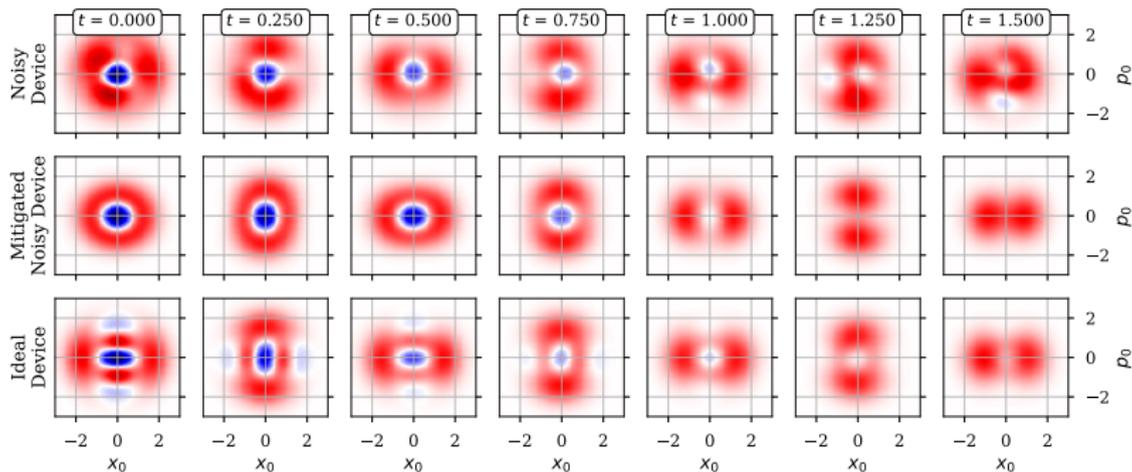


(Results obtained on the IonQ Harmony Quantum Device, June 2024)

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



Questions

Scan to download these slides:



<https://cburdine.github.io/files/srnl.pdf>

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

Acknowledgments

- **Dr. Julia Y. Chan's Lab** (Baylor University)
 - Superconductor Synthesis
- **Nora Bauer and Dr. George Siopsis**
(University of Tennessee Knoxville)
 - Collaborators, Access to Quantinuum Hardware at ORNL
- IonQ and Microsoft Azure Quantum
 - Access to Quantum Hardware, Compute Credits
- **Dr. Enrique P. Blair** (Baylor University)
 - Advisor, Mentor, Collaborator

Thank you for your time and consideration!

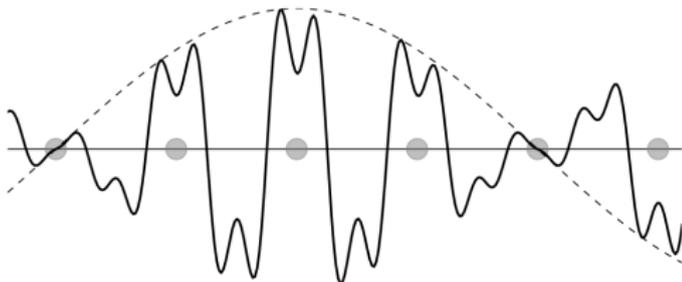
My website: <https://cburdine.github.io>

Additional Slides and References

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} :

$$\hat{H}(\vec{k}) = \sum_{i,j \in (\text{cell})} e^{i\vec{k}\cdot(\vec{r}_i - \vec{r}_j)} \tilde{h}_{ij} \hat{c}_i^\dagger \hat{c}_j \quad (5)$$

Representing Atomic Orbitals

- Solving for the crystal's allowed electron energies requires diagonalizing the matrix representation of $\hat{H}(\vec{k})$ for each possible \vec{k} .
- The effective Hamiltonian coefficients \tilde{h}_{ij} can be approximated as

$$\tilde{h}_{ij} = \langle \phi_i | V(r) | \phi_j \rangle = \int \phi_{n_i}^*(\vec{x} - \vec{r}_i) V(r) \phi_{n_j}(\vec{x} - \vec{r}_j) d\vec{x} \quad (6)$$

- 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:

$$X'_{\ell,c}(r, \theta, \varphi) = i^{n_c} \sqrt{\frac{2\pi}{2\ell+1}} r^\ell [Y_{\ell,m}(\theta, \varphi) \pm Y_{\ell,-m}(\theta, \varphi)] \quad (7)$$

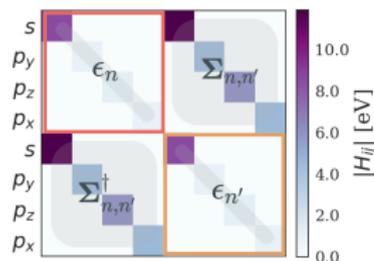
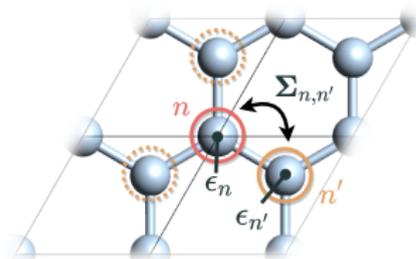
(Above, we use $c = \ell + m$, where \pm denotes $\text{sign}(m)$ and $n_c \in \{0, 1, 2, 3\}$)

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

$$F(r), V(r) \propto \sum_{s=1}^{N_s} c_s e^{-\alpha_s r^2} \quad (8)$$

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 $\Sigma_{n,n'}$:

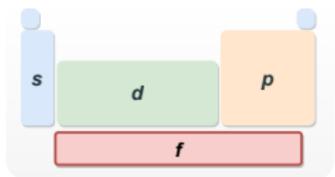


- The matrix $\mathbf{H}(\vec{k})$ can be diagonalized for each \vec{k} to obtain eigenvalues (**the band structure**) and eigenvectors (**the Bloch orbitals**).

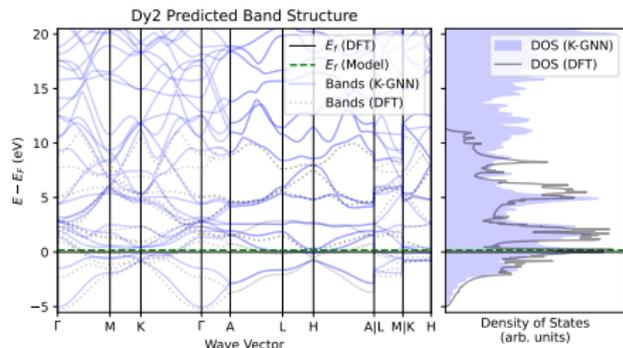
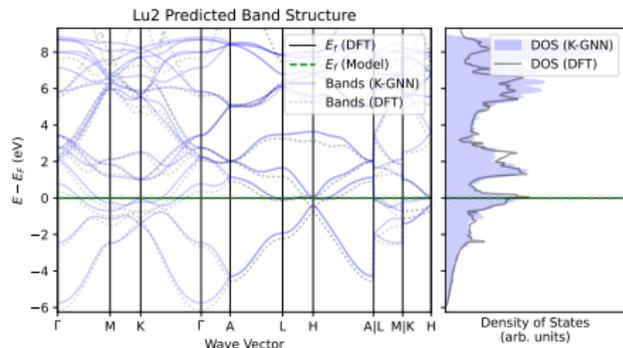
More about QuINNs

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.



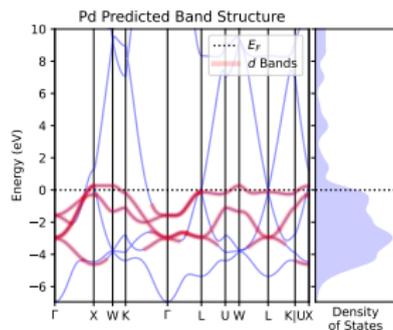
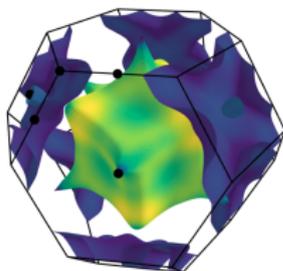
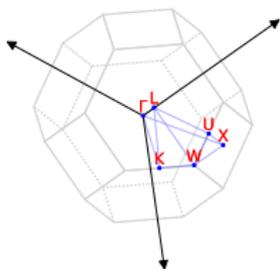
- However, QuINNs have limited capacity to capture conducting states accurately for heavy atoms.



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

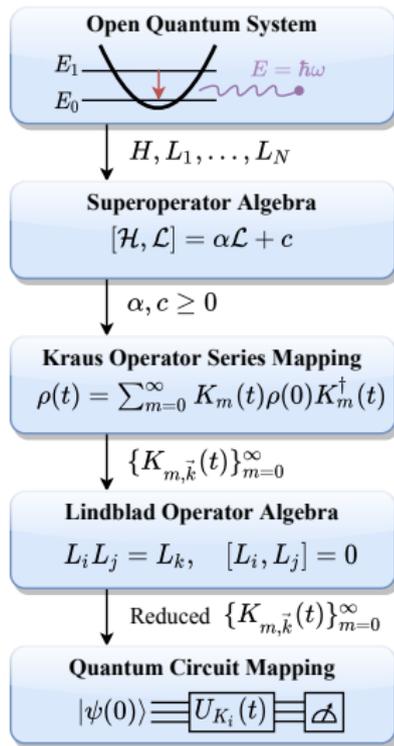
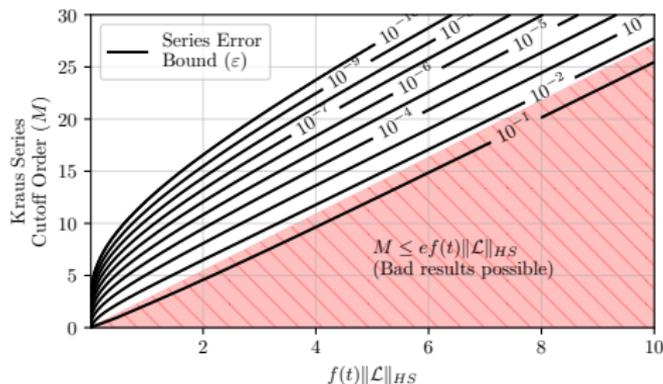


Simulation of Open Quantum Systems

The Time-Perturbative Kraus Series Method

- Our method expands the evolution of ρ as a 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.
- We proved asymptotically linear scaling of M with evolution time t :



Future Work

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



QUANTINUUM

- Future directions to explore include:
 - Generalizing the time-perturbative Kraus series method to estimate observables via randomly sampled circuits.
 - Characterizing the kinds of systems where our method yields an exponential quantum advantage.
 - Exploring hardware-aware error mitigation techniques to improve simulation fidelity.

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