

Predictive Modeling in High-Temperature Superconductors: Comparative Insights from Density Functional Theory and Machine Learning

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Abstract. Superconductivity, defined by the disappearance of electrical resistance below a critical temperature, holds significant promise for future technologies such as quantum computing, maglev transport, and energy-efficient power grids. Among the many superconducting materials, nickel and copper oxide stand out due to their comparable layered structures but distinct electronic properties. Understanding and predicting their superconducting behavior is essential for discovering new high-temperature superconductors. Density functional theory and machine learning have become indispensable tools in this effort. While DFT offers insights into band structure and orbital interactions, ML models enable high-throughput screening of potential materials. However, data scarcity, model interpretability, and limited generalizability remain significant barriers to progress. This review critically evaluates the effectiveness and limitations of these predictive techniques, identifies unresolved issues, and discusses integrative research strategies that combine theory, simulation, and experimentation to accelerate discoveries in high-Tc superconductivity. This comparative analysis offers a roadmap for building interpretable, efficient, and scalable predictive models in the next phase of high-Tc materials research.

Keywords: superconductivity, nickel oxide, copper oxide, density functional theory (DFT), machine learning (ML).

1. Introduction

Superconductivity is a quantum phenomenon where materials exhibit zero electrical resistance below a critical temperature (Tc). Since the discovery of copper oxide superconductors in the 1980s [1], high-temperature superconductivity (HTS) has attracted considerable research attention due to its potential applications in quantum computing, power transmission, and magnetic levitation. Among known HTS materials, copper oxides and the more recently discovered nickel oxides have become key research targets due to their unique crystal structures and complex electronic interactions.

Both families feature layered perovskite-like structures, with CuO_2 or NiO_2 planes believed to be responsible for superconducting behavior [2]. However, their electronic structures and mechanisms differ in essential ways. Copper oxides exhibit strong antiferromagnetic fluctuations and a well-established 'pseudogap' phase, while nickelates remain under investigation, with their pairing mechanisms not yet fully understood. Predictive methods such as DFT and ML have increasingly explored these differences and accelerated materials discovery. This paper reviews and compares recent research on the application of these methods, highlighting their strengths, limitations, and potential for identifying new superconductors. We focus on copper and nickel oxides because they present a compelling case for comparative analysis. Despite their shared structural motifs, they exhibit notably different superconducting mechanisms, making them ideal candidates for testing the predictive capabilities of various computational tools. Copper oxides are well-established, data-rich systems with known properties, providing a reliable baseline.

In contrast, nickelates are emerging materials that challenge existing models and expose limitations in current theoretical and data-driven frameworks. Similarly, density functional theory (DFT) and machine learning (ML) are chosen not only for their growing prevalence in materials research, but also for their contrasting epistemological strengths—DFT offers interpretable, physics-based modeling, whereas ML enables scalable, pattern-based prediction. By comparing their performance across these two material families, this review aims to assess where each method succeeds or falls short, and to propose strategies for combining their strengths in future research on high-temperature superconductivity.

2. Definition and Properties of Nickel Oxide and Copper Oxide Superconductors

2.1 Crystal Structure

Both copper oxides (cuprates) and nickel oxides (nickelates) adopt layered perovskite-like structures, where the superconductivity is believed to originate within two-dimensional CuO_2 or NiO_2 planes. These planes are typically separated by charge reservoir layers, influencing doping and carrier concentration. A hallmark example is $YBa_2Cu_3O_7$ (YBCO), where CuO_2 planes are stacked with BaO and Cu-O chains, leading to robust superconducting behavior. Similarly, in nickelates such as $NdNiO_2$, the infinite-layer structure mirrors that of the cuprates, with rare-earth spacer layers replacing charge reservoirs [3]. This structural resemblance has fueled interest in nickelates as potential analogs to cuprates. However, despite these similarities, subtle differences—such as bond lengths, cation coordination environments, and lattice instabilities—can strongly affect electronic properties and superconductivity.

2.2 Electronic Structure

The electronic configurations of cuprates and nickelates differ substantially. Cuprates exhibit strong electron correlations and a half-filled $3d^9$ configuration in Cu^{2+} ions, giving rise to Mott insulating behavior in undoped states. Their Fermi surfaces and electronic structures evolve dramatically with doping, often passing through a pseudogap phase. In contrast, nickelates like $NdNiO_2$ feature a nominally similar $3d^9$ configuration, yet exhibit more itinerant behavior, weaker correlation effects, and a less well-defined Mott gap [3, 4]. Recent DFT+DMFT calculations suggest that nickelates may host orbital-selective correlations, with 3d orbitals exhibiting different localization degrees depending on strain or chemical pressure [4]. The absence of a robust pseudogap and the lack of long-range magnetic order in nickelates distinguish their electronic landscape from that of cuprates.

2.3 Superconducting Mechanism

The superconducting mechanisms in cuprates and nickelates remain an area of active investigation, with significant contrasts. Cuprates display a d-wave pairing symmetry, likely mediated by antiferromagnetic spin fluctuations, and exhibit a rich phase diagram that includes the pseudogap, strange metal, and superconducting states. This well-established phenomenology has guided decades of theoretical work. Nickelates, however, challenge this understanding. Their superconductivity emerges without clear signatures of a pseudogap or spin fluctuation-dominated regime. For instance, in the infinite-layer nickelate $Nd_{1-x}Sr_xNiO_2$, superconductivity appears near a quantum critical point without an accompanying antiferromagnetic order [2]. This suggests a different pairing mechanism—possibly involving enhanced hybridization between Ni 3d and rare-earth 5d orbitals or subtle charge-transfer physics.

2.4 Experimental Maturity and Materials Challenges

Cuprates benefit from decades of synthesis refinement and extensive characterization. Their critical temperatures can exceed 90 K, and thin-film growth techniques, such as pulsed laser deposition and molecular beam epitaxy, are well established. In contrast, nickelates remain synthetically challenging. Stabilizing infinite-layer phases requires topotactic reduction of perovskite precursors under carefully controlled conditions [5]. The metastability of these phases, their sensitivity to oxygen content, and the difficulty of achieving epitaxial strain complicate reproducibility. Nevertheless, the successful synthesis of $La_3Ni_2O_7$ under high pressure and its observed spin-density-wave transition have broadened the scope of nickelate-based superconductivity, pointing to a rich phase space yet to be fully explored.

2.5 Similarities and Differences

Cuprates and nickelates share a common structural motif but differ markedly in electronic behavior, pairing mechanisms, and experimental maturity. While both possess layered architectures and involve 3d transition metals in square planar coordination, their superconducting states emerge from distinct physical origins. Cuprates are better understood, with a wealth of data supporting spin-mediated pairing, whereas nickelates present a frontier for testing new models and refining predictive tools. These contrasts make them ideal complementary systems for evaluating the strengths and limitations of computational approaches like DFT and ML.

3. Evaluation of Predictive Methods

3.1 Density Functional Theory (DFT) and Extensions

Density Functional Theory is widely used to study the ground-state properties of solids. While effective in weakly correlated systems, standard DFT falls short in high-temperature superconductivity due to strong electron-electron interactions. For example, in copper oxides, standard DFT often incorrectly predicts a metallic state, whereas experiments reveal Mott insulating behavior in the undoped limit. This limitation stems from DFT underestimating on-site Coulomb repulsion, which affects orbital occupations and band gaps. In nickelates, the challenge is subtler: while metallic behavior may be correctly predicted, standard DFT cannot fully capture the orbital-selective correlations and valence fluctuations observed experimentally [3].

Extensions such as DFT+U and DFT+DMFT have been employed to address these issues. DFT+U adds a Hubbard U term to represent localized electrons better and has successfully reproduced insulating states and Fermi surface evolution in cuprates like $YBa_2Cu_3O_7$ [4]. DFT+DMFT, incorporating time-dependent local correlations, has improved accuracy in modeling mixed valence behavior and orbital differentiation in nickelates [3]. For instance, in $NdNiO_2$, DFT+DMFT captures the influence of rare-earth orbitals and the suppression of magnetic order under doping.

These approaches, however, are computationally demanding and sensitive to input parameters such as U values and double-counting corrections. In many cases, choices regarding how to treat rare-earth f-electrons and oxygen vacancies introduce uncertainty. Recent progress to mitigate these challenges includes self-consistent U determination, high-throughput DFT workflows with uncertainty quantification, and machine learning surrogates to accelerate screening while preserving physical accuracy.

Nickel oxide's potential is further underscored by its applications in functional electronic devices such as sensors and transistors, as outlined in [6]. It indicates that its complex behavior holds implications beyond superconductivity alone. Furthermore, material fabrication challenges—such as forming stable infinite-layer nickelates—remain a barrier to reproducibility and large-scale integration [5]. Understanding how structural strain and pressure alter superconducting states is critical, and recent studies have shown that applying high pressure can significantly modulate spin-density-wave transitions, which may correlate with superconductivity [5].

Studies have also explored the importance of ceramic coatings and heterostructures in improving thermal and chemical stability, particularly relevant for high-Tc superconductor applications where environmental sensitivity is an issue [7]. These findings suggest that interface and surface engineering advances may play a significant role in enhancing the robustness of superconducting materials.

Overall, while DFT remains a foundational tool for exploring the electronic structure of superconductors, its predictive power in correlated oxides is limited without methodological refinement or empirical calibration.

3.2 Machine Learning Models

Machine learning offers a data-driven alternative to first-principles approaches such as DFT. ML models can identify patterns and rapidly predict previously unstudied materials by training on established datasets. Most models in superconductivity research use supervised learning techniques, where input features like composition, electronegativity, and atomic radii are mapped to target properties like critical temperature or stability.

Standard algorithms include neural networks, decision trees, and support vector machines. For example, on test data, Lee et al. developed a neural network model that predicted the Tc of cuprates with an RMSE of approximately 10–15 K [8]. Such models enable high-throughput screening of candidate materials, significantly reducing the time and cost of identifying promising superconductors.

A key advantage of ML is its ability to manage high-dimensional feature spaces and uncover non-linear correlations that are difficult to model with physics-based approaches. This capability allows researchers to explore large chemical spaces and prioritize candidates for further DFT or experimental validation. ML has also been used to predict other material properties, such as thermodynamic stability, electronic bandgap, and formation energy, enabling pre-screening without complete quantum calculations.

However, ML models depend heavily on the availability and quality of training data. Many high-Tc superconductors are complex and sensitive to synthesis conditions, leading to noisy or inconsistent data across different studies. In addition, the “black box” nature of many ML models makes them difficult to interpret, limiting their value for understanding underlying physical mechanisms.

Both DFT and ML approaches face limitations. DFT struggles with dynamic and non-local correlations, while ML models require extensive, high-quality data and often lack interpretability. Additionally, most studies focus on bulk properties, whereas real-world applications demand understanding of thin films, interfaces, and defects.

Limited experimental data hampers model training and validation for nickelates. Moreover, differences in synthesis conditions and measurement techniques introduce noise into databases. Bridging the gap between theory and experiment requires better models, standardized datasets, and protocols.

To mitigate these challenges, researchers have adopted explainable AI techniques, such as SHAP, which stands for Shapley Additive explanations, to identify which features drive model predictions. Active learning strategies have also improved data efficiency, where models iteratively select the most informative new data points. Furthermore, incorporating physically meaningful descriptors, such as orbital character or coordination number, can enhance interpretability and generalizability.

4. Limitations and Future Directions

4.1 Future Directions

One particularly promising area is the exploration of hydrogen-rich materials. Notably, Drozdov et al demonstrated superconductivity at 250K in lanthanum hydride under high pressures, pushing the boundary of achievable in-room-temperature superconductivity [9]. This opens avenues for investigating other light-element-based compounds that may mimic similar electron-phonon coupling mechanisms.

In parallel, graph neural networks (GNNs) such as CGCNN and MEGNet are gaining attention due to their ability to directly encode crystal structures as graphs and predict materials' properties with high fidelity. These methods have significantly improved accuracy over classical ML models, especially in energy and electronic property prediction, and are increasingly applied in superconductor screening tasks.

Additionally, integrating theoretical predictions with socio-political frameworks can ensure that research priorities align with public interest and policy constraints. However, inaccurate, transferable models hindered previous modeling efforts, especially in correlated systems like nickelates. Many ML models trained on cuprates failed to generalize due to electronic structure differences, while DFT required parameter tuning and was sensitive to input approximations.

Several strategies could improve the predictive modeling of High Temperature Superconductivity such as: integrating physics-based simulations with ML to retain interpretability while enhancing scalability, iteratively refining ML models by selecting the most informative data points from simulations or experiments, encouraging publication of negative results and synthesis conditions to enrich datasets, using explainable AI tools to identify which features influence superconductivity predictions and combining insights from condensed matter physics, materials chemistry, and computer science.

These developments suggest a shift toward integrated, intelligent discovery pipelines that couple simulation, learning, and experiment. By embedding recent advances in ML and automation, researchers can accelerate the discovery of high-Tc materials while mitigating the limitations of previous one-method approaches.

4.2 Broader Implications

High-temperature superconductors have already demonstrated significant advantages for power systems. For instance, HTS-based AC cables offer high current capacity, reduced energy losses, and compact size, making them well-suited for urban electrical grids [10]. The Holbrook Superconductor Project in New York exemplifies the successful deployment of superconducting power cables in real-world infrastructure [11].

However, despite their potential, many proposed superconductors have not been commercialized due to limitations in durability, cost, and compatibility with manufacturing processes. Early-stage research often prioritized properties like Tc while ignoring other critical parameters such as mechanical stability, chemical robustness, and manufacturability. For example, ceramic coatings for enhanced thermal stability—critical for deployment in complex environments—were often overlooked in early modeling efforts, but are now being actively investigated [7].

HTS materials are also used in fault current limiters, energy storage, and magnetic shielding. Agencies such as the U.S. Department of Homeland Security are considering them for their potential to improve grid resilience [12]. As energy systems transition to sustainable sources, HTS can play a pivotal role in enhancing the reliability and efficiency of future smart grids.

In quantum computing, superconducting qubits are currently one of the most scalable and controllable architectures [13]. Companies like IBM and Google have built processors using Josephson junction-based superconducting circuits. These systems benefit from high coherence times and the ability to implement fast quantum logic gates.

These applications emphasize that HTS research should aim for high Tc and current density and consider material durability, cost-effectiveness, and integration feasibility. The synergy between DFT, ML, and materials informatics can help prioritize high-performance, manufacturable, and environmentally viable candidates. Integrating DFT and ML into materials informatics pipelines enables the identification of new superconductors by performance, sustainability, and manufacturability.

5. Conclusion

This review has examined and compared two major predictive approaches—density functional theory (DFT) and machine learning (ML)—in studying high-temperature superconductors, focusing on copper and nickel oxides. While DFT provides deep physical insight into electronic structure and correlation effects, its accuracy is often constrained by parameter sensitivity and high computational cost. Conversely, ML enables rapid prediction and large-scale screening but faces interpretability and data quality challenges.

These limitations have hindered understanding complex systems such as nickelates, where experimental data is limited and theoretical models are difficult to validate. However, recent advances—including graph neural networks, active learning, and self-supervised representations—are bridging these gaps. Hybrid approaches integrating DFT-calculated features with ML-based inference offer new pathways for discovering scalable and interpretable materials.

Looking forward, the success of high-Tc superconductor research will depend not only on improving predictive accuracy but also on aligning modeling strategies with synthesis constraints, environmental considerations, and practical deployment. By combining computational physics, data science, and experimental feedback, the field is entering a more integrated and application-driven era of superconductor design.

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