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Predictive Modelling of Electronic Materials: A Review of Deep Learning Techniques in Computer Engineering

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ABSTRACT

This review evaluates the application of deep learning (DL) for the predictive modeling of electronic materials in computer engineering. We analyzed peer-reviewed literature across four major databases, focusing exclusively on advanced architectures like Graph Neural Networks (GNNs) and Generative models. Results indicate these models accurately predict critical properties, such as band gaps and thermal conductivity, for next-generation semiconductors, 2D materials, and memristors. These high accuracies are achieved because architectures like GNNs effectively capture complex 3D spatial interactions without requiring manual feature engineering. However, practical fabrication remains hindered by data scarcity, algorithmic opacity, and a profound "Sim-to-Real Gap". While DL accelerates predictive design, sustaining Moore's Law ultimately requires developing autonomous "Self-Driving Labs" and Large Material Models to bridge digital predictions with physical synthesis.

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1. INTRODUCTION

The continuous evolution of computer engineering relies heavily on the rapid discovery and integration of novel electronic materials to sustain the performance scaling historically dictated by Moore's Law (Lundstrom & Alam, 2022). As traditional silicon-based architectures approach their fundamental physical and thermal limitations, there is a critical and immediate need for advanced semiconductors, two-dimensional (2D) materials, and components suitable for neuromorphic computing (Liu *et al.,* 2020). Historically, the discovery and optimization of these critical computing materials have depended heavily on slow, trial-and-error laboratory experiments or computationally expensive *ab initio* calculations (Gomes *et al.,* 2019). Specifically, conventional computational methods such as Density Functional Theory (DFT) provide high atomic-level accuracy but suffer from severe scalability issues when applied to the complex crystalline structures required for next-generation microelectronics (Jain *et al.*, 2022). Consequently, this computational bottleneck poses a significant challenge, significantly delaying the deployment of new hardware solutions that are necessary for emerging technologies like quantum computing and energy-efficient edge architectures, thereby hindering innovation cycles, increasing development costs, and limiting scalability across modern digital ecosystems (Fuhr and Sumpter, 2022).

To overcome these fundamental limitations, data-driven approaches, particularly Deep Learning (DL), have recently emerged as a transformative paradigm in computational materials science (Merchant *et al.*, 2023). State-of-the-art research has demonstrated that advanced neural network architectures, such as Graph Neural Networks (GNNs) and Generative Adversarial Networks (GANs), can predict complex material properties orders of magnitude faster than traditional quantum mechanical simulations (Dai *et al.*, 2021). Recent empirical studies have successfully utilized these DL frameworks to predict the band gaps of novel semiconductors, optimize the thermal conductivity of heat-dissipating materials, and design high-k dielectrics for advanced transistors (Li *et al.*, 2025; Choudhary *et al.*, 2021). However, despite the rapid proliferation of DL applications in general materials discovery, most existing review literature broadly addresses general materials science without specifically targeting the stringent, application-specific requirements of computer engineering (Schmidt *et al.*, 2019). Furthermore, previous reviews often conflate traditional machine learning algorithms with DL, thereby diluting the specific advancements made by deep representation learning in microchip design and Electronic Design Automation (EDA) (Batzner *et al.*, 2022). Therefore, a critical gap exists in systematically synthesizing how modern DL architectures specifically accelerate the predictive modelling of electronic materials tailored exclusively for computing hardware (Sánchez *et al.*, 2023). This paper provides novelty by isolating DL models and directly bridging their predictive capabilities with the practical material demands of contemporary computer architecture, offering a hardware-centric perspective that is currently absent in the literature (Altman *et al.*, 2024).

The primary objective of this review is to systematically evaluate the application of DL techniques in the predictive modelling of electronic materials strictly within the context of computer engineering. This paper aims to elucidate how various DL architectures, particularly GNNs and transformer-based foundational models, are utilized to predict the electrical, thermal, and structural properties essential for manufacturing next-generation hardware components. The scope of this review is carefully limited to research published within the last decade, focusing exclusively on materials directly applicable to semiconductor manufacturing, emerging non-volatile memory technologies, and brain-inspired computing architectures. By comprehensively mapping the current landscape of DL-driven material discovery, this paper intends to provide researchers and hardware engineers with a detailed roadmap of current capabilities, lingering challenges such as dataset scarcity, and future directions for autonomous hardware design.

2. METHODS

This systematic review was conducted to evaluate studies at the intersection of artificial intelligence, computational materials science, and computer engineering. The literature search targeted four major academic databases: IEEE Xplore, Scopus, Web of Science, and the ACM Digital Library. Specific Boolean keyword strings focusing on DL, electronic materials, and predictive modelling were utilized to isolate highly relevant research. The criteria strictly required studies to utilize advanced DL architectures such as GNNs, Convolutional Neural Networks (CNNs), or Generative models with direct applications to computer and electronic engineering. Consequently, research relying on shallow machine learning algorithms (e.g., Random Forests) or addressing unrelated material domains (e.g., biomaterials) was excluded. During data extraction, the selected papers were systematically categorized along two primary dimensions. First, they were classified by the specific DL architecture employed. Second, they were grouped by the type of electronic material targeted, such as next-generation semiconductors, 2D materials, or memristive materials.

3. RESULTS AND DISCUSSION

This section delineates the principal findings from contemporary literature regarding the application of DL in the discovery and optimization of electronic materials. By analyzing the types of materials investigated, the predictive architectures employed, and the performance metrics achieved, a comprehensive understanding of the current landscape is established. Furthermore, this section critically examines the prevailing limitations that continue to challenge researchers in the field.

3.1. Electronic Material Categories in Computer Engineering

The current trajectory of DL-driven materials discovery is fundamentally motivated by the need to transcend the physical limitations of silicon-based architectures and sustain the progression of Moore's Law. To achieve this, researchers are heavily focusing on next-generation wide-bandgap semiconductors, which are essential for developing high-power and high-frequency computing applications (Merchant *et al.*, 2023). Beyond traditional bulk semiconductors, there is a profound interest in 2D materials, such as graphene and Transition Metal Dichalcogenides (TMDs). Because these materials can be scaled down to an atomic thickness, they are highly sought after for ultra-scaled field-effect transistors. Machine learning models are now extensively deployed to predict the complex phase stability and electronic doping effects inherent to these 2D structures (Abdulazeez & Ageed, 2024).

Concurrently, the microprocessing industry faces severe challenges regarding quantum tunnelling and leakage currents as transistor nodes shrink. Consequently, the search for novel high-k dielectric materials has been significantly accelerated by DL-based predictive modelling, which minimizes the traditional reliance on exhaustive trial-and-error experimentation (Islam, 2024). Finally, as the computing paradigm expands beyond classical von Neumann architectures, transition metal oxides exhibiting memristive properties are being rigorously explored for neuromorphic computing. In this domain, DL has proven invaluable in identifying precise elemental combinations that yield the optimal on/off resistance ratios required to mimic biological synapses (see **Table 1**).

Table 1. Categorization of electronic materials in computer engineering and DL prediction targets.

MATERIAL CATEGORY	APPLICATION IN COMPUTER ENGINEERING	PROMINENT EXAMPLES	PRIMARY DL PREDICTION TARGET
Next-Generation Semiconductors	High-power/high-frequency processors, Power electronics	SiC, GaN, ZnO	Bandgap, Carrier mobility, Thermal conductivity
2D Materials	Ultra-scaled Field-Effect Transistors (FETs), Interconnects	MoS_2, Graphene, WSe_2	Phase stability, Carrier mobility, Doping effects
High-k Dielectrics	Gate insulators in advanced processors, Memory capacitors	HfO_2, ZrO_2, Al_2O_3	Dielectric constant (k-value), Leakage current prevention
Memristive Materials	Neuromorphic chips (artificial synapses), Non-volatile memory	TiO_2, TaO_x, HfO_x	On/off resistance ratio, Switching endurance, Conductance states

3.2. DL Architectures in Predictive Modelling

The efficacy of predicting material properties is intrinsically tied to how the material data is represented and the specific neural network architecture chosen to process it. Historically, CNNs established the standard for computer vision tasks within materials science. They are still predominantly utilized to extract nuanced features from microstructural imagery, such as Scanning Electron Microscopy, or from 2D and 3D voxel grids. This capability enables the automated detection of crystallographic defects that could severely degrade processor performance (Abdulazeez & Alnabi, 2024; Hasan, 2022).

However, as the field has advanced, GNNs have emerged as the state-of-the-art approach for modelling crystalline and molecular structures. By representing atoms as nodes and chemical bonds as edges, frameworks like Crystal Graph Convolutional Neural Networks can effectively capture complex 3D spatial interactions and local chemical environments without requiring manual feature engineering (Abdulazeez & Hasan, 2025; Abdullah *et al.*, 2025). While GNNs and CNNs excel at forward predictive modelling, the introduction of Generative Models has facilitated a paradigm shift toward inverse design. Variational Autoencoders, GANs, and Transformer-based architectures now empower AI to generate entirely novel, unsynthesized crystallographic blueprints that are mathematically optimized for specifically targeted computational properties (Goodfellow *et al.*, 2020) (see **Figure 1**).

3.3. Predicted Properties and Performance Metrics

An evaluation of recent computational literature reveals that DL regression metrics are increasingly approaching the accuracy of *ab initio* DFT calculations, yet they operate at a mere fraction of the computational cost. Naturally, the prediction of electronic properties, specifically band gaps and electrical conductivity, constitutes the bulk of this research. Recent GNN ensembles have demonstrated remarkable precision, often predicting band gaps with a deviation of less than 0.1 eV from experimental validations (Sánchez *et al.*, 2023; Ahmed *et al.*, 2024).

Beyond purely electronic behavior, thermal management remains a critical bottleneck in high-performance computing. To address this, DL models have been successfully adapted to predict the thermal conductivity of materials, aiding in the design of advanced, highly efficient processor cooling layers (Abo-Zahhad *et al.*, 2022). Ultimately, however, a material is only as useful as its physical viability. Therefore, before physical synthesis, these models are rigorously applied to predict formation energy and hull distance. This critical step ensures that the generated materials are thermodynamically stable and will not structurally degrade under normal operating temperatures (see **Figure 2**).

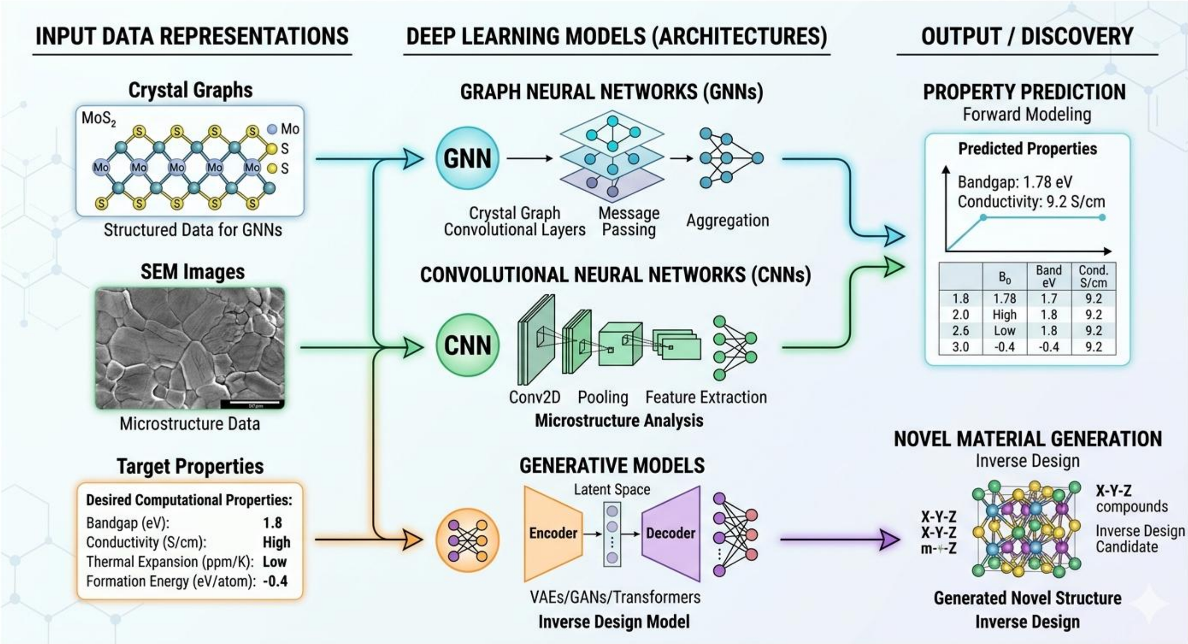

Figure 1. Architectural framework of DL models applied in the discovery and optimization of electronic materials.

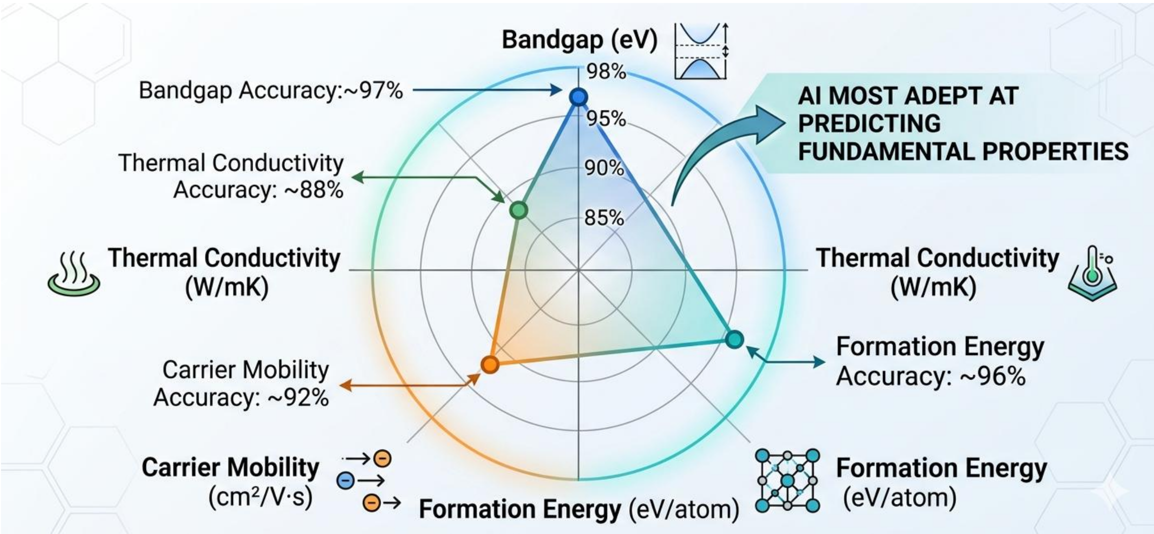

Figure 2. DL performance for electronic material properties.

3.4. Current Challenges and Limitations

Despite the massive progress observed in predictive accuracy, the seamless integration of DL into electronic materials science is currently constrained by several fundamental bottlenecks. The most pressing of these is data scarcity. Unlike Natural Language Processing, which benefits from trillions of training tokens, high-quality empirical materials data is exceptionally limited. Existing large-scale databases are primarily populated by computationally derived DFT data rather than empirical experimental results, which frequently introduces theoretical biases into the predictive models.

Furthermore, the inherent "black-box" nature of advanced DL models obscures the physical and chemical mechanisms driving their predictions. This lack of interpretability generates understandable hesitancy among physicists and hardware engineers, who require mechanistic reasoning and physical proofs before investing in the fabrication of new chip materials. Consequently, this leads to a profound "Sim-to-Real Gap." A significant disparity exists between computational prediction and real-world synthesis; an AI-generated semiconductor might exhibit exceptional theoretical properties *in silico*, yet prove to be completely unsynthesizable in a physical fabrication plant due to complex thermodynamic or kinetic constraints that the algorithm failed to capture (Jain *et al.*, 2022) (see **Figure 3**).

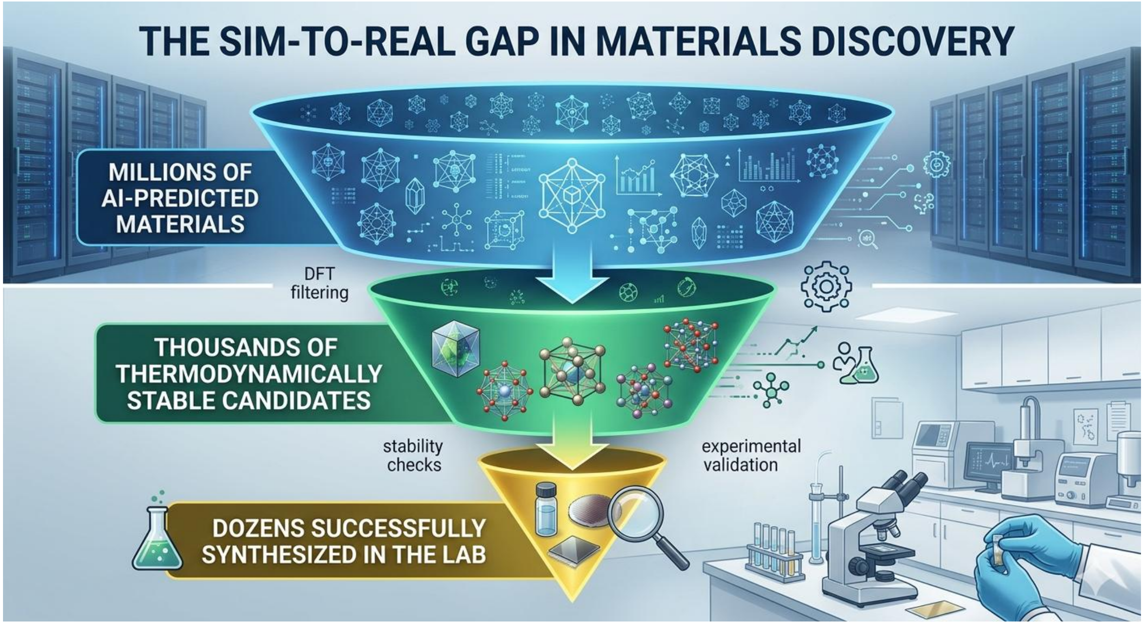

Figure 3. SIM-to-real gap in materials discovery.

3.5. Future Directions

Based on the trajectory of current literature, the future of electronic materials research will inevitably shift from isolated computational predictions toward fully autonomous, intelligent discovery ecosystems. Central to this vision is the development of Large Material Models (LMMs). Drawing inspiration from the unprecedented success of Large Language Models, future research will pivot toward multimodal Foundation Models specifically engineered for materials science. These robust networks will be trained concurrently on diverse datasets, including scientific literature, topological molecular graphs, and time-series characterization data. Ultimately, this integration could enable computer engineers to use simple natural language prompts to instantly generate viable, ready-to-synthesize material blueprints.

To bridge the gap between these digital blueprints and physical reality, the convergence of DL and advanced robotics will catalyze the era of "Self-Driving Labs." In this autonomous paradigm, AI algorithms will act as the central nervous system, formulating chemical recipes and directing robotic arms to perform the physical synthesis. These robotic systems will subsequently conduct real-time characterization and feed the empirical data directly back into the model for continuous learning. By establishing this closed-loop system, the scientific community will be able to drastically accelerate the empirical validation of predicted materials, effectively resolving the data scarcity and sim-to-real bottlenecks that currently define the field (see **Figure 4**).

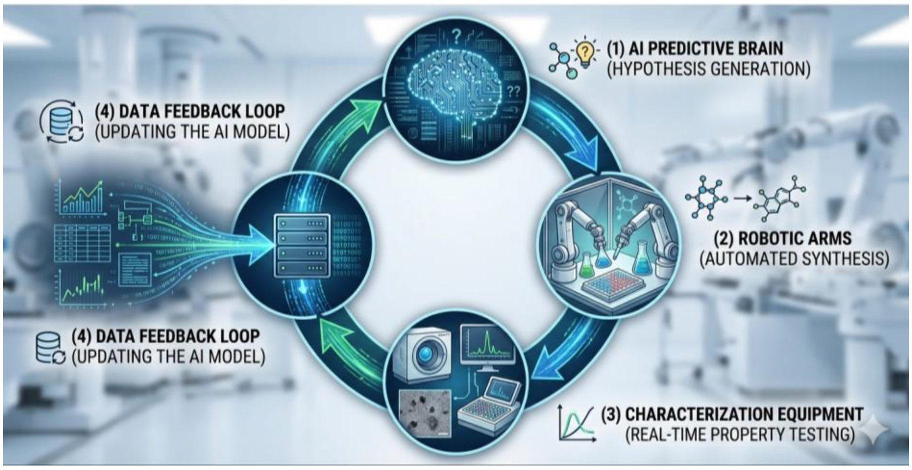

Figure 4. The self-driving lab concept: A closed-loop cycle for autonomous material discovery.

4. CONCLUSION

DL has transformed electronic material discovery from trial-and-error experimentation to accelerated predictive design. Architectures like GNNs and Generative Models accurately predict properties for next-generation semiconductors, 2D materials, and memristors at a fraction of traditional computational costs. However, practical implementation remains hindered by data scarcity, algorithmic opacity, and a profound "sim-to-real gap" where theoretically viable materials fail physical synthesis. Ultimately, bridging this digital-to-physical gap requires developing LMMs and autonomous "Self-Driving Labs." By integrating predictive AI with automated robotic synthesis, DL will drive future high-performance computing hardware and sustain Moore's Law.

5. AUTHORS' NOTE

The authors declare that there is no conflict of interest regarding the publication of this article. The authors confirmed that the paper was free of plagiarism.

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