

REVIEW

Open Access



# A critical review on electronic materials properties and multifunctional applications

Wubshet Getachew Mengesha<sup>1\*</sup> and Kaveer Nagessar<sup>2</sup>

\*Correspondence:

Wubshet Getachew Mengesha  
wubshet2003@gmail.com

<sup>1</sup>Department of Physics, Woldia  
University, Woldia, Ethiopia

<sup>2</sup>Department of Physics, University  
of Pretoria, Pretoria, South Africa

## Abstract

The rapid advancement of electronic technologies necessitates the development of materials with tailored properties for multifunctional applications. However, there are significant challenges include a fundamental gap in connecting quantum-level behavior to macroscopic properties, data scarcity, and difficulties in integrating multidisciplinary datasets. This paper aims to analyze recent advancements and propose integrated frameworks to bridge these gaps by leveraging artificial intelligence (AI) and machine learning (ML) with a comprehensive review methodology and critical analysis of properties, types, their diverse applications coupled with AI-driven approaches, including generative models, physics-informed neural networks, and autonomous laboratories, for predicting and optimizing electronic materials. Key findings highlight their diverse applications and discovery such as perovskites, 2D materials, and high-temperature superconductors—and in optimizing electronic, thermal, and magnetic characteristics. Recent studies indicate that AI-driven approaches can improve prediction accuracy and enable inverse design in selected systems. These approaches have the potential for significant impact on materials discovery and integration, potentially leading to a transformation of the electronic materials landscape. This paper underscores the future potential of AI-driven paradigms to revolutionize the electronic materials landscape by integrating computational prediction with experimental validation for multifunctional real-world applications.

**Keywords** Electronic materials, Materials discovery, Multifunctional applications, Quantum materials, Artificial intelligence, Machine learning

## 1 Introduction

The quest for new electronic materials—the building blocks of everything—has long been a meticulous process of trial and error for investigating a material with the desired properties for a specific or multifunctional applications. The development of advanced electronic materials has traditionally relied on iterative experimental approaches and computationally intensive simulations. Scientists have long faced challenges in predicting how specific atomic configurations will manifest in macroscopic material properties, particularly for multifunctional applications that require balancing multiple performance metrics such as conductivity, thermal stability, and scalability [1, 2]. Foundational



© The Author(s) 2025. **Open Access** This article is licensed under a Creative Commons Attribution-NonCommercial-NoDerivatives 4.0 International License, which permits any non-commercial use, sharing, distribution and reproduction in any medium or format, as long as you give appropriate credit to the original author(s) and the source, provide a link to the Creative Commons licence, and indicate if you modified the licensed material. You do not have permission under this licence to share adapted material derived from this article or parts of it. The images or other third party material in this article are included in the article's Creative Commons licence, unless indicated otherwise in a credit line to the material. If material is not included in the article's Creative Commons licence and your intended use is not permitted by statutory regulation or exceeds the permitted use, you will need to obtain permission directly from the copyright holder. To view a copy of this licence, visit <http://creativecommons.org/licenses/by-nc-nd/4.0/>.

computational methods like Density Functional Theory (DFT) provide valuable theoretical insights but remain limited in their ability to efficiently explore vast chemical spaces due to their significant computational costs [3, 4]. These limitations have driven the development of new methodologies that can bridge theoretical predictions with experimental validation. By integrating insights from both computational simulations and empirical data, researchers are creating more holistic prediction pipelines that can decode the complex relationships between atomic structure and material properties [5, 6]. This integrated approach has proven particularly valuable in the discovery and optimization of novel material classes, including perovskites for photovoltaics, two-dimensional materials for electronics, and advanced superconductors for quantum technologies [6–8].

Despite these advances, significant challenges persist. Data scarcity remains a fundamental constraint, with high-quality experimental data often limited and difficult to obtain [9]. Furthermore, the integration of multidisciplinary datasets from diverse sources and experimental techniques presents substantial obstacles to developing unified predictive frameworks [10, 11]. Perhaps most critically, there exists a fundamental gap in connecting quantum-level electronic behavior, including quantum transport phenomena and carrier dynamics, with macroscopic material properties and performance metrics [12, 13]. Addressing these challenges requires the development of new approaches that can effectively incorporate physical constraints and principles into predictive models. By integrating multi-fidelity data that combines both approximate and high-precision measurements, researchers aim to create more robust frameworks for material discovery and optimization [14]. The ultimate goal is to enable the design of materials with tailored functionalities specifically engineered for particular applications, whether for enhanced photovoltaics, flexible electronics, or quantum computing devices. This paper aims to analyze recent advancements in electronic materials development, identify persistent challenges in data integration and model development, and propose frameworks for connecting fundamental electronic behavior with practical material performance. By establishing stronger connections between quantum mechanical principles, predictive modeling, and experimental validation, we can advance toward more sustainable and scalable innovation in next-generation electronic materials [15–17].

Modern scientific discovery increasingly depends on the seamless integration of theoretical models, advanced computational techniques, experimental validation, and AI-driven approaches, forming a synergistic framework that accelerates the development of novel materials and devices, as illustrated in Fig. 1. This integration allows researchers to leverage the predictive power of simulations, the empirical accuracy of experiments, and the pattern-recognition capabilities of AI to explore vast design spaces more efficiently than traditional methods alone. The graphical abstract, (2), illustrates the transformative evolution in electronic materials research from traditional approaches to an AI-driven discovery paradigm.

Figure 2, depicts a comprehensive research framework progressing from fundamental principles through materials taxonomy to multifunctional applications, with artificial intelligence serving as the central accelerator across all domains. Traditional methods including DFT calculations and experimental trial-and-error are evolving into advanced AI methodologies such as physics-informed neural networks, generative models, and autonomous laboratories. This AI-enhanced framework addresses persistent challenges

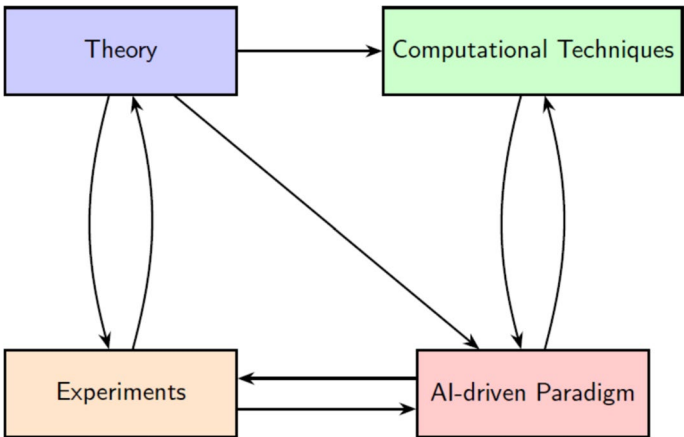


**Fig. 1** Synergistic integration of theoretical models, computational methods, experimental validation, and AI-driven approaches, illustrating how these components collectively accelerate scientific discovery

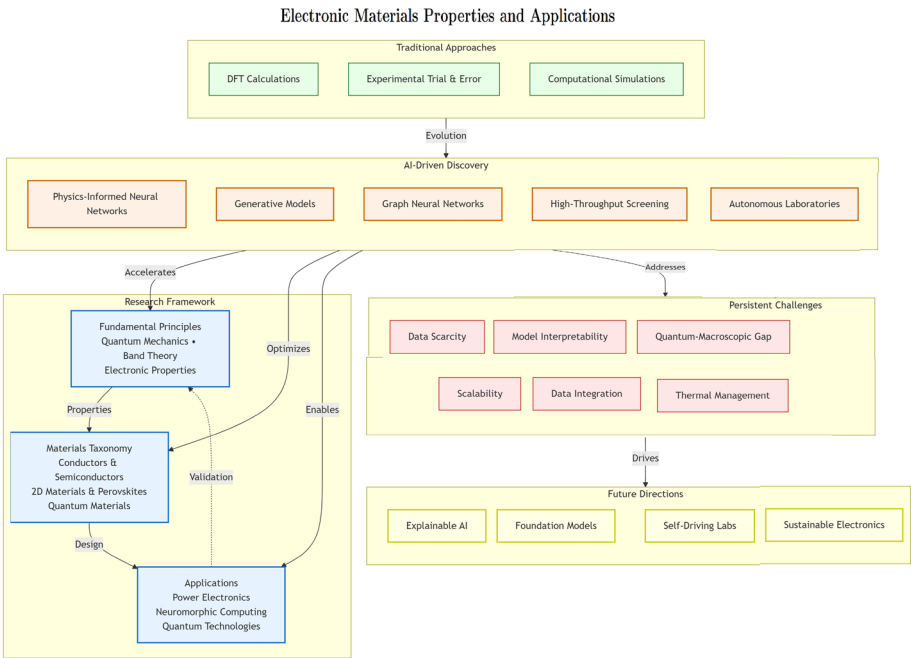


**Fig. 2** Graphical abstract illustrating the electronic materials discovery, showcasing the evolution from traditional methods to an integrated workflow that connects fundamental principles, materials taxonomy, and multifunctional applications while addressing key challenges and future directions

including data scarcity, the quantum-macroscopic gap, and thermal management, while driving future directions toward explainable AI, foundation models, and sustainable electronics. The integrated workflow demonstrates how AI-driven prediction and optimization enable tailored material design for advanced applications in power electronics, neuromorphic computing, and quantum technologies, creating a continuous innovation cycle from fundamental discovery to practical implementation.

This paper comprehensively examines the field of electronic materials through four interconnected sections that progress from fundamental principles to cutting-edge applications and future perspectives. The next section describes AI and Machine Learning Methodologies, the next section concerned with the theoretical foundation

of electronic materials, exploring quantum mechanical principles, band theory, and key electronic properties. It covers quantum transport phenomena, dielectric behavior, semiconductor physics, and band engineering strategies that enable tailored material functionalities. In the fourth section, a comprehensive taxonomy of electronic materials organized by their fundamental properties and applications has been described. It covers conductors, semiconductors, dielectrics/insulators, magnetic materials, piezoelectric/ferroelectric materials, wide-bandgap semiconductors, 2D materials, polymers, and composites. The classification is supported by equations, figures and a table. The fifth section explores the practical implementation of electronic materials across diverse technological domains. It examines power electronics, optoelectronics, imaging technologies, multifunctional sensing devices, memory systems, neuromorphic computing, thin-film transistors, and spintronics. Supporting figures and a table provide visual comparisons of material performance metrics, device characteristics, and application-specific requirements. The final section presents a critical analysis of current advancements, persistent challenges, and future research trajectories. It highlights AI-driven materials discovery, autonomous laboratories, and emerging applications in quantum computing and sustainable electronics.

Having outlined the introduction part with the transformative potential of integrated approaches in electronic materials research, we now delve into the specific artificial intelligence and machine learning methodologies that are instigating this paradigm shift.

## 2 AI and machine learning methodologies for electronic materials

The integration of artificial intelligence (AI) and machine learning (ML) is instigating a paradigm shift in electronic materials research, moving beyond traditional, intuition-driven approaches to create powerful, data-centric discovery and design pipelines. These methodologies are not merely incremental improvements but represent a fundamental change in how we explore complex chemical spaces, predict multifaceted properties, and design novel functional materials from the atom up [18–20]. This section provides a detailed overview of the core AI/ML architectures driving this transformation, explaining their underlying principles, specific strengths, and illustrative applications in electronic materials.

**Physics-informed neural networks (PINNs):** A primary constraint in applying ML to novel material systems is the scarcity of high-quality, curated experimental data. Physics-Informed Neural Networks (PINNs) directly address this limitation by integrating the governing physical equations—expressed as partial differential equations directly into the learning process [21, 22]. This is achieved by incorporating the PDE residuals into the neural network's loss function, penalizing solutions that violate known physical laws. This paradigm ensures predictions are not merely statistical fits but, significantly enhancing generalizability and reducing dependency on massive datasets. In electronic materials, PINNs excel in simulating electromagnetic phenomena by embedding Maxwell's equations, enabling the rapid and accurate design of nanophotonic devices, meta-optics, and antenna systems [23]. Their application extends to electronic design automation (EDA), where they facilitate robust device modeling and circuit optimization under uncertainty, ensuring performance and reliability [24].

**Generative models:** A transformative application of AI is *inverse design*: specifying a target property and allowing an algorithm to generate the corresponding material

structure. Generative Adversarial Networks (GANs) are particularly powerful for this task. A GAN consists of two competing neural networks: a generator that creates candidate structures from a latent space, and a discriminator that evaluates their authenticity against a training set of real materials [25, 26]. Through this adversarial training, the generator learns to produce increasingly realistic and novel designs. Notable implementations include Crystal GAN for discovering complex metal hydrides for energy storage, and MatGAN/CubicGAN for generating novel, chemically valid inorganic crystals with high success rates [18–20]. Conditional GANs further refine this by generating structures (e.g., nanophotonic components) directly from a target optical response [27]. This approach has been extended to design architecture materials with tailored mechanical properties, generating microstructures that approach theoretical elastic limits [28, 29].

**Graph neural networks (GNNs):** Crystalline and molecular materials are inherently graph-structured with atoms as nodes and bonds as edges—GNNs provide a natural and powerful representation [30, 31]. GNNs operate by passing messages (feature vectors) between connected nodes, allowing each atom's representation to be informed by its local chemical environment. This architecture excels at capturing complex, non-local dependencies that determine electronic and thermal properties. Specialized GNN architectures have become the gold standard for property prediction. The Crystal Graph Convolutional Neural Network (CGCNN) directly operates on the crystal graph to predict formation energies and band gaps, while the Atomistic Line Graph Neural Network (ALIGNN) incorporates bond angles by using the line graph of the crystal graph, achieving remarkable accuracy in predicting vibrational and thermal properties [32–34]. Beyond global properties, GNNs can predict local behaviors like atomic stress distributions, enabling the design of atomic structures with optimized performance for specific electronic or mechanical applications [35].

**Reinforcement Learning (RL)** frames material design as a sequential decision-making process. An agent learns to make optimal choices (e.g., selecting a molecular fragment or a synthesis parameter) by interacting with an environment (a simulation or a lab), receiving rewards for actions that lead to improved target properties [36, 37]. This paradigm is exceptionally valuable for optimizing complex, multi-step processes where a clear objective exists but large labeled datasets are unavailable. RL has demonstrated significant success in diverse domains: the organic model designs novel, high-melting-point organic molecules, RL agents have been used to design polymer sequences that maximize thermal conductivity, and they can create bioinspired composite microstructures that reduce stress concentrations. In electronics, RL frameworks have been deployed for analog circuit optimization, autonomously converging on circuit designs that meet target specifications significantly faster than traditional genetic algorithms [18, 24, 38].

**Hybrid and integrated frameworks:** The most powerful and promising future direction lies in hybrid frameworks that synergistically combine multiple AI methodologies. These integrated systems leverage the strengths of individual models to overcome their respective limitations. For instance, the Self-Adaptable Graph Attention Network with Symbolic Regression (SA-GAT-SR) combines the high predictive accuracy of a GNN with the human interpretability of symbolic regression, distilling complex structure–property relationships into compact, analytical.

equations [34]. Other advanced systems integrate reinforcement learning with evolutionary algorithms for robust optimization, transformers for forecasting temporal

synthesis data, and quantum-inspired generative models for exploring complex multi-objective landscapes [39]. The field is rapidly evolving towards multi-modal generative models that can process diverse data types (e.g., text, spectra, images) and fully autonomous "self-driving" laboratories. These closed-loop systems integrate AI-driven prediction, robotic synthesis, and automated characterization, creating a continuous cycle of hypothesis generation and testing that heralds a new era of accelerated innovation [40, 41].

**Practical workflows from high-throughput screening to generative design:** These AI methodologies are deployed in powerful computational workflows. ML-enabled high-throughput screening uses hierarchical strategies, where fast, low-fidelity ML models (e.g., classical force fields or simple GNNs) screen millions of candidates to identify a small pool of promising leads for subsequent validation with high-fidelity, computationally expensive DFT calculations. This has been successfully applied to screen thousands of 2D materials for electronic applications and to identify stable, lead-free hybrid perovskites for photovoltaics from libraries of over 5,000 candidates [42, 43]. Data-driven frameworks systematically identify promising material classes, such as novel transparent conductors, while multi-task learning frameworks simultaneously predict multiple properties from a shared representation, dramatically reducing the computational cost per property [44–46]. Ultimately, these approaches are coalescing into automated pipelines that dramatically accelerate the entire electronic materials discovery and design timeline, from initial concept to realized device [47, 48].

Equipped with an understanding of the core AI/ML architectures driving modern discovery, we next establish the essential theoretical foundation of electronic materials, exploring the quantum mechanical principles and electronic structure that govern their behavior.

### 3 Fundamental principles in electronic materials

Electronic materials, substances engineered to control the flow of electrons for conduction, insulation, or semi-conduction, are governed by quantum mechanics, solid-state physics, and materials chemistry. Quantum mechanics dictates conductivity, band structures, and electromagnetic interactions, with recent advances focusing on nanoscale property manipulation. Band theory, central to electron energy-level descriptions, underpins breakthroughs in topological insulators and 2D materials such as graphene, enabling novel electronic behaviors. The increasing demand for batteries and compact electronics is driven by their high energy density and excellent power-to-mass ratio. However, challenges such as uneven temperature distribution, inefficient energy storage, and slow-release rates have emerged. To ensure optimal performance and longevity of these devices, effective heat dissipation is essential, highlighting the need for thermally conductive hybrid fillers to enhance thermal management [12, 49–51].

Key innovations in electronic materials have emerged from advancements in several critical areas, including quantum transport, dielectric enhancements, semiconductor physics, and band engineering. Each of these domains contributes significantly to the development of next-generation electronic devices.

#### 3.1 Innovations in electronic materials

Key Innovations and Characteristics have described in the following parts:

**Quantum transport:** Quantum transport explores the behavior of the charge carrier at the quantum level, critical for nanoscale electronics. AI-driven atomic simulations and ML models enable precise predictions in 2D materials such as TMDs, optimizing carrier mobility and defect tolerance. High-throughput screening with DFT identifies quantum-coherent materials for computing, while large language models like *Honey Bee* accelerate discovery [52, 53].

**Dielectric enhancements:** Dielectric materials are vital for capacitance and energy storage. The polyG2G model, for example, has generated novel polymer dielectrics with targeted permittivity, achieving a >15% improvement in certain performance metrics over known baselines [54, 55].

**Semiconductor physics:** Advances include 2D materials and topological insulators for low-power devices. AI frameworks like Joint Automated Repository for Various Integrated Simulations (JARVIS) predict properties (e.g., bandgap) using ML-trained DFT datasets. Bayesian deep learning enables inverse design of ultra-wide bandgap semiconductors (GaN, AlScN), while autonomous labs integrate AI-driven synthesis [56–58].

**Band engineering:** Adjusting band structures via alloying, strain, or quantum wells tailors electronic properties. Transfer learning adapts predictions across material classes, and hybrid AI optimizes band alignment in catalytic/thermoelectric systems. Diffusion models and Explainable AI (XAI) enable tunable bandgaps and structure–property insights [12, 13, 59].

The synergy of quantum transport, dielectric enhancements, semiconductor physics, and band engineering drives next-generation electronics and quantum technologies. AI accelerates discovery by predicting crystal structures and material stability, combining quantum simulations with ML [60].

### 3.2 Band theory and electronic structure

Band theory is crucial for understanding the behavior of electrons in solids. Computational frameworks powered by artificial intelligence can efficiently calculate band structures and state density, providing deeper insights into material performance under varying conditions. Such approaches allow researchers to optimize materials for improved electrical performance. Band theory underpins the understanding of electronic materials and describes how electrons occupy energy levels in solids. Recent studies have used artificial intelligence to predict the band structures and electronic properties of complex materials, including 2D semiconductors and perovskites [61, 62]. The electrons in an atom are occupied in certain regions or atomic states orbiting around the nucleus, which have a certain range of energies forming electron energy bands, or bands for short. Each type of material has a slightly different configuration for these states. In certain solids, the bands can overlap, while there can be a gap between two adjacent bands known as a band gap. The two important bands in semiconductors are the valence and conduction bands. The valence band is the outermost band filled with electrons that do not move freely, while in the conduction band, electrons are loosely bound to the atom and move freely. Electrons in the conduction band result in the material conducting electricity. Metals can conduct because of the overlapping of the valence and conduction bands. A semiconductor can also be defined as having a band gap of less than 2 eV; however, certain semiconductors have band gaps of 2–7 eV with niche applications. The band structure (i.e., its energy–momentum or E-k relationship) of the

crystal ultimately determines several properties of the material. The atoms in the crystal interact with each other, causing forces of attraction and repulsion that will balance out. Taking many atoms into account affects the band structure of the material. The three-dimensional Schrodinger equation with one electron can be solved to find this energy–momentum relationship. Bloch’s theorem is one of the most important theorems about band structure. DFT calculations reveal that doping  $\text{Ge}_2\text{Sb}_2\text{Te}_5$  with  $\text{Co}_2\text{FeAl}$  reduces  $E_g$  from 0.7 to 0.3 eV, enhancing interfacial spin polarization [63]. AI-driven band structure aligns with the angle resolved photoemission spectroscopy (ARPES) data within 5% error [64].

### 3.3 Electrical, thermal and magnetic characteristics

Electrical conductivity ( $\sigma$ ) is a fundamental property governed by the mobility and concentration of the charge carrier. Artificial intelligence (AI) models are increasingly employed to elucidate the complex relationships between a material’s microstructure and its resulting conductivity. These AI-driven insights are critical for guiding the development of high-performance conductors, transistors, and interconnects [60, 65]. Furthermore, machine learning techniques are leveraged to optimize key processes such as doping and defect engineering, and to identify novel materials exhibiting optimal ionic conductivity for advanced battery applications [66, 67]. The application of advanced neural network potentials enables the high-fidelity simulation of charge dynamics at the atomic scale, providing unprecedented detail into transport phenomena [68].

Dielectric and magnetic properties are paramount for the functionality of capacitors, memory devices, and spintronic systems. AI significantly accelerates the discovery pipeline for materials with tailored permittivity ( $\epsilon_r$ ) and specific magnetic responses [69, 70]. ML models demonstrate proficiency in predicting complex magnetic ordering and in the computational design of polymers with high dielectric strength. The integration of ML extends to the parameterization of fundamental physical models; for instance, the Jiles–Atherton model for magnetic hysteresis can be accurately parameterized using ML techniques to capture the nuanced behavior of magnetic cores [71].

Thermal and optical properties are decisive in applications involving light-matter interactions and thermal management. AI-based predictive frameworks are used to accurately determine thermal conductivity ( $k$ ) in complex nanostructures and to optimize the composition of plasmonic materials for enhanced performance in photovoltaics [72, 73]. Neural networks are also deployed to forecast thermal transport behavior and to aid in the rational design of materials with engineered bandgaps, which is essential for the development of efficient LEDs and photodetectors [65, 74, 75].

Having established the fundamental quantum mechanical principles and electronic structure properties that govern material behavior, we now systematically categorize the diverse landscape of electronic materials. This classification organizes materials by their dominant charge transport mechanisms and functional responses, providing a structured framework for understanding their respective roles in modern technology.

## 4 Electronic material types

The emergence and proliferation of nanotechnology have served as a primary catalyst for transformative progress within the electronics sector and, by extension, the broader information society. This technological revolution has facilitated the creation of devices

that are not only significantly miniaturized but also exhibit superior computational speed, enhanced energy efficiency, and greater portability. Consequently, these advanced systems possess an unprecedented capacity for processing, managing, and storing vast quantities of data, fundamentally reshaping modern technological capabilities.

#### 4.1 Batteries, resistors and capacitors

Batteries are indispensable for energy storage and portable electronics. They operate on the basis of electrochemical reactions that store and release electrical energy through ion movement between electrodes (anode and cathode) via an electrolyte. Modern battery technologies include lithium-ion, sodium-ion, magnesium-ion, and solid-state batteries, each with unique advantages and challenges. Resistive materials are fundamental components in electronic circuits. AI has been used to model resistive switching behaviors in memristors, enabling their application in neuromorphic computing [76].

Resistors are categorized by construction and materials. Wire wound resistors use nickel–chromium alloy wires wound around ceramic/fiberglass cores with enamel coatings. Carbon composition resistors (CCR) combine carbon particles with conductive ceramics, while film resistors deposit materials like carbon, nichrome, tantalum nitride (metal film), or tin oxide (metal oxide) onto insulating cores. Foil resistors employ metallic foils for precision [77]. N-type semi-conductive GaAs could be used as resistor material and is manufactured in a manner similar to a field effect transistor (FET) [78]. AI optimizes alloy compositions for stability and high-permittivity capacitor polymers, while ML-driven additive manufacturing tailors wire geometries to minimize resistive losses [79]. AI further ensures precise resistivity control during fabrication. GANs optimize Cr-Si thin-film resistors for temperature coefficients of resistance ( $\text{TCR} < 10 \text{ ppm/K}$ ) [80].

Capacitive materials, such as graphene-barium titanate composites, have been fabricated and characterized using low-temperature processing techniques. AI aids in optimizing their performance for energy storage applications [81]. Capacitors store charge via conductive plates separated by dielectrics. Air capacitors use metallic plates with air gaps, while ceramic, electrolytic, and supercapacitors leverage advanced materials like carbon nanotubes or graphene for high charge storage, sustainability, and wide operational ranges [82–84]. High-permittivity ceramics/polymers, enhanced through doping strategies [85], are widely used. Ab-initio and DFT-ML studies model supercapacitors with carbon, boron, and titanium [86–88]. Robotics driven by AI synthesizes components, and ML predicts the resistivity of the alloy. ML identifies  $\text{ZrO}_2\text{-HfO}_2$  nanolaminates as high- $\kappa$  dielectrics ( $\epsilon_r > 40$ ) with breakdown fields  $> 8 \text{ MV/cm}$  [89, 90].

#### 4.2 Semiconductors

Semiconductor devices benefit from AI-driven optimizations in material selection and device architecture. Flexible memristors, for example, have been developed for advanced computing and sensing applications, showcasing the versatility of AI in semiconductor research [91]. The behavior of semiconductor devices needs to be studied, as certain devices in devices include multiple layers of different semiconductors, doping levels, and defects. Semiconductor devices include diodes, transistors, thyristors, and optoelectronic devices. When two semiconductor materials are placed together, a junction is formed along with a depletion region, where no free charge carriers exist.

This region controls the flow of current and allows conduction under certain conditions. This mechanism is widely used in many semiconductor devices. An example of a junction is the p–n junction seen in most diodes or the metal–semiconductor junction formed in Schottky diodes. Semiconductors form the backbone of modern electronics. They are essential for transistors and integrated circuits and enable controlled electrical conduction.

AI techniques facilitate the optimization of semiconductor interfaces, defect engineering, and doping profiles, leading to improved transistor reliability. AI optimizes device performance by analyzing doping effects, defects, and surface interactions. Machine learning guides the fabrication of high-speed silicon transistors and generates synthetic microstructures to enhance solar cell charge transport [92–94]. Physics-informed neural networks refine transistor doping profiles, while AI accelerates the design of battery cathodes and photovoltaic materials [95–97].

PINNs model phase transitions in GeSbTe-based memristors, achieving 10 ns switching speeds. For instance, AI-driven defect engineering in SiC power devices reduces leakage currents by 40% compared to traditional methods [98, 99]. Phase-change materials (e.g., Ge–Sb–Te alloys) benefit from AI-driven simulations of switching kinetics for non-volatile memory [100]. AI also identifies next-generation semiconductors, such as lead-free perovskites and MXenes [101, 102], advancing sustainable, high-efficiency technologies. Further DFT and ML studies are needed to accurately model semiconductor devices.

The most common semiconductor materials are Silicon (Si), Gallium Arsenide (GaAs), Gallium Nitride (GaN), Germanium (Ge), and Silicon Carbide (SiC). Silicon is the most widely used semiconductor material and is a IV semiconductor that has many applications in photovoltaics, microelectromechanical systems (MEMS) electronic devices and integrated circuits. Silicon can be p-type when doped with boron and n-type if doped with elements such as antimony, arsenic, and phosphorous. Most silicon wafers are made from the Czochraski method. Silicon has a cubic structure that is covalently bonded. Silicon is hard but brittle material and has a band gap of 1.12 eV. [103]. When silicon is highly doped, as the temperature increases, the band gap of silicon decreases by the following Varshni formula.

$$E_g(T) = E_g(0) - \frac{\alpha T^2}{(T + \beta)} \quad (1)$$

with  $E_g(T)$  being the final energy band gap,  $E_g(0)$  being the energy band gap at 0 K, with material constants for silicon being  $\alpha = 4.730 \times 10^{-4} \text{ eV K}^{-1}$  and  $\beta = 636 \text{ K}$ . [104].

Gallium arsenide is a III-V semiconductor that has applications in modern optoelectronics and high-speed electronics. It has application in the making of laser diodes and is used often in space applications as a Schottky barrier diode (SBDs). GaAs has a cubic zincblende structure and GaAs single crystals are extremely brittle. GaAs has a band gap of 1.42 eV which can be extended by alloying it to Aluminum to get something of the form  $Al_xGa_{1-x}As$ . GaAs gas is a direct band gap which means that in the transition between the valence a band maximum and conduction band minimum, there is no momentum change and thus there is no particle interaction to occur and hence the two energy levels align with respect to momentum [105, 106]. GaN and SiC and other similar compound semiconductors like AlGaN and InGaN are a wide-band gap semiconductors

often used in light-emitting diodes and other optoelectronic applications. They both have the ability to work in high temperature and high-power applications [107–111]. Germanium can be used like GaN and SiC in optoelectronics and has applications in microelectronics when combined with Silicon in a CMOS device [112, 113].

There is an exhaustive list of semiconductive materials of which DFT, Machine-Learning and AI could be used to find new materials to model defect and the effect of doping in the crystal lattice of these semiconductors, which can alter their properties. DFT has been applied with the most common semiconductors. AI and machine learning can assist in getting more consistent results across semiconductors. Boron Nitride is one of the least understood wide- band gap semiconductor and is considered as a possible photonic and energy storage material [114–118]. Diamond is also considered a wide band gap semiconductor with high carrier mobility and thermal conductivity, despite being an expensive material. Diamond devices increase power performances at high temperatures [119, 120]. Ab-initio DFT studies have concluded that Beryllium-Sulfur (*BeS*)-doped graphene could be a viable transistor material on the basis of its optical properties. The electronic ground state of *BeS* has been studied by other groups [121, 122]. Further experimentation and the use of machine learning techniques are needed be used to study *BeS* as a wide-band gap semiconductor.

Figure 3 presents a comparative analysis of semiconductor properties. It shows the temperature dependence of Silicon's band gap, calculated using Eq. (1). The band gap decreases from approximately 1.16 eV at 0 K, with a dashed line indicating the room temperature value of 1.12 eV. The bar chart presents a comparing band gap energies of various semiconductor materials at room temperature, categorized as: IV Semiconductors (Si, Ge), III-V Semiconductors (GaAs, GaN), and Wide Bandgap materials (SiC, BN, Diamond). Band gap values increase substantially across these categories, with Diamond and BN exhibiting the largest band gaps exceeding 5 eV.

A research team used a Deep Adaptive Regressive Weighted Intelligent Network (DARWIN) to predict that a class of materials of the form  $K_2CuX_3$  (with  $X = Cl$  or  $Br$ ) as a promising semiconductor family, based on its electronegativity difference. A other group took a list of quaternary semiconductor compositions and used microgravimetric methods to find four candidates with direct bandgaps. DFT was then used to analyze the electronic properties of these quaternary semiconductors and verified the conclusions of ML and found other unique electrical proper- ties [123]. Graph-based neural networks

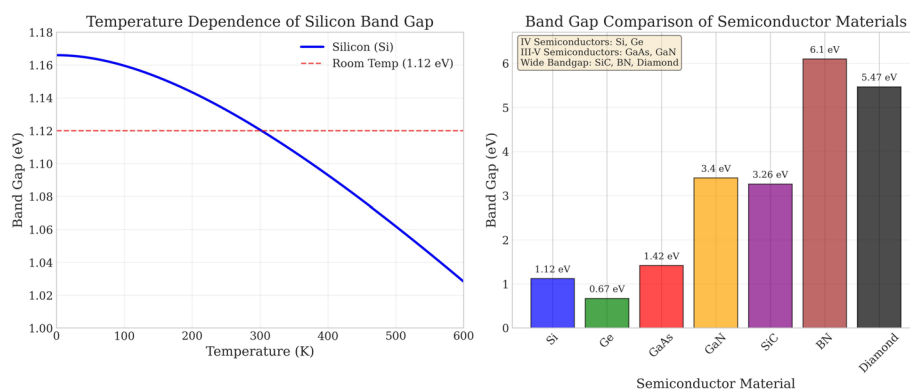


**Fig. 3** A comparative analysis of semiconductor properties based the temperature dependence of Silicon's band gap

have been used to predict defect formation energies in the chemical space of zinc blend semiconductors [124, 125]. Several other studies have verified that ML and AI help and accelerate utilization when calculating semiconductor properties [126, 127].

#### 4.3 High-temperature superconducting materials

Superconductors transport electrical charges without resistance, magnetic fields are pushed out from the interior, and exhibit various macroscopic quantum phenomena. They have significant practical applications especially in the revolutionization of the energy industry, as superconducting wires and electrical systems may transport and deliver electricity with no energy loss [128–130]. Discovering new superconductors remains a grand challenge. AI platforms analyze vast chemical spaces to identify potential high-temperature superconductors, significantly reducing experimental trial-and-error efforts. Superconductive materials can be classified into two types. Type I are completely diamagnetic during the superconducting state due to the Meissner effect and include Aluminum, Lead, Tin, and Mercury. Type II superconductors are diamagnetic at a low applied magnetic field and include materials like Niobium-Zirconium (Nb-Zr) alloys, Niobium-Titanium (Nb-Ti) alloys, and  $Nb_3Sn$ . Iron-based superconductors, particularly FeSe, are pivotal for efficient energy transport and high-field magnets. Strategies like elemental substitution, pressurization, and electron doping enhance critical temperatures ( $T_c$ ), revealing unconventional superconductivity mechanisms. Sparse modeling identifies lattice strain as a key descriptor in cuprates, while deep learning accelerates heavy fermion superconductor discovery [131, 132]. AI further optimizes compositions for high-temperature superconductivity. AI models predict superconducting transitions and optimize material compositions for high-temperature superconductors, advancing their use in power transmission and quantum technologies. This is exemplified by ML models that screened over 12,000 cuprate compositions to identify high-temperature superconductors, a task that would be prohibitively slow using DFT alone [133, 134].

#### 4.4 Ceramics, polymers, carbon-based materials

Polymers are large molecules composed of many repeating subunits called monomers. Electrical polymers can be thought of as semiconductors and quasi-particle charge carriers have been proposed to explain how polymers conduct [135, 136]. Ceramic materials are compounds between metallic and nonmetallic elements and include conductive ceramics like tin oxide, zirconium oxide, silicon carbide, and molybdenum disilicide [137]. Carbon nanomaterials are seen as new and advanced materials. Further studies are required to understand the conduction mechanism in ceramics, polymers and carbon-based materials. AI-driven evolutionary algorithms design stretchable conductive polymers for wearables, and deep learning inspires bioinspired spiderweb-inspired composites [138, 139]. Convolutional Neural Networks (CNNs) predict ceramic crack propagation for aerospace use, while ML optimizes polymer dielectrics and carbon composites [95, 140, 141]. Data-driven models reduce lattice thermal conductivity in ceramics, and carbon-based materials (e.g., graphene) excel in electrical or thermal performance [142, 143]. Ceramics, polymers, and carbon-based materials exhibit diverse functionalities. AI accelerates the discovery of novel compositions and architectures, such as conductive polymer composites for thermoelectrics [73]. AI predicts mechanical, electrical, and thermal properties of ceramics, polymers, and carbon-based materials, enabling

breakthroughs in lightweight composites and flexible electronics. Reinforcement learning designs porous SiC ceramics for 99% EMI shielding at 30 GHz. CNT-reinforced epoxy composites achieve  $k = 6.2$  W/mK via AI-optimized alignment [60, 144, 145].

#### 4.5 Two-dimensional (2D) electronic materials

Two-dimensional (2D) materials represent a class of substances defined by their atomic-scale thickness and typically exhibit surfaces free of dangling bonds. This fundamental characteristic has driven immense research interest, primarily due to their perfectly planar geometry, a suite of distinctive physical properties, and their extensive potential for integration into various device platforms [60, 146, 147]. This family of ultrathin materials encompasses a diverse range of compounds, including graphene, transition metal dichalcogenides (TMDs), hexagonal boron nitride (h-BN), and MXenes. Their unique electronic structure, exceptional optical characteristics, and superior mechanical flexibility underpin their critical role in enabling significant progress across multiple technological domains. These applications are vast and include high-performance semiconductors, highly sensitive sensors, next-generation energy storage systems, efficient catalysts, and pioneering quantum technologies, as extensively documented in the literature [93, 148–152]. AI-driven workflows are revolutionizing the design and discovery of 2D materials. For instance, ML has been used to guide the strategic adsorption on novel dumbbell monolayers, simultaneously optimizing electronic transport and suppressing thermal conductivity to maximize thermoelectric performance [153]. Beyond property optimization, ML is critical for navigating vast, unexplored chemical spaces, as demonstrated by its integration with traditional methods to rapidly screen thousands of hypothetical 2D carbon nitride structures for stability and catalytic potential [154].

A paramount advantage of 2D materials is the highly tunable nature of their intrinsic properties. This tailoring can be achieved through a variety of sophisticated engineering strategies, such as applying precise strain, inducing controlled phase transitions, introducing specific defects, modifying surface chemistry, stacking different numbers of layers, and forming van der Waals heterostructures by vertically assembling disparate 2D crystals. This extensive adaptability makes them exceptionally suitable for the design and fabrication of next-generation electronic and optoelectronic devices [155]. Furthermore, the field is increasingly leveraging artificial intelligence to accelerate the discovery and application of these materials. Advanced computational techniques, including deep learning, transfer learning, and generative models, are now routinely employed to predict complex electronic structures with high accuracy, simulate properties that vary with layer number, rapidly screen vast chemical spaces for stable new materials, and rationally design optimal heterostructures with desired functionalities. This powerful synergy between AI and materials science is significantly expediting the development cycle and facilitating the seamless integration of 2D materials into advanced functional devices, as demonstrated by numerous recent studies [59, 156–162].

#### 4.6 Perovskites

Perovskites are materials with a crystal structure of the form  $ABC_3$ , where A represents a monovalent or divalent cation (e.g. Cs or Ca), B is typically a transition metal such as Fe, and C can be an oxide or a halide. Their unique structures and adaptable optoelectronic properties make them pivotal in photovoltaics, optoelectronics, spintronics, and

catalysis [163–165]. Renowned for tunable band gaps, high charge mobility, and excellent light absorption, these materials excel in solar cell applications, driving significant improvements in power conversion efficiency. The ability to integrate perovskites with flexible substrates and scale production underscores their potential in advancing renewable energy solutions and developing better solar cells for niche applications. Similarly, 2D materials complement these efforts by offering innovative functionalities in electronics and energy storage, further enhancing the technological landscape.

AI is revolutionizing perovskite development by tackling performance and stability simultaneously. It enables multi-objective optimization, screening for ideal band gaps alongside synthesizability and formability [166]. Furthermore, AI guides defect passivation, discovers lead-free variants, and even designs self-healing layers to significantly extend operational lifetime [138, 167–169]. Halide perovskites, known for their soft lattice and tunable band structure, enable diverse applications in photovoltaics, LEDs, optoelectronics, and X-ray detectors, with recent advancements extending their use to microelectronics like artificial synapses and resistive memories [142, 170]. Perovskite research has made remarkable progress due to AI-guided synthesis routes that enhance stability and efficiency. Surface engineering strategies have led to record-breaking performance in solar cells. GAN-generated  $\text{CH}_3\text{NH}_3\text{PbI}_3$  variants achieve 25% photovoltaic efficiency with defect tolerance  $\eta > 10^{16} \text{ cm}^{-3}$  [62, 64, 171].

#### 4.7 Quantum materials

The fundamental properties and behaviors of all materials are intrinsically governed by the principles of quantum mechanics, which provide the foundational framework for understanding atomic bonding, electronic interactions, and collective phenomena at the most elementary level. A specific class of substances, known as quantum materials, has emerged as a subject of intense research due to their ability to exhibit pronounced quantum–mechanical effects across remarkably extended energy and length scales, often persisting even at elevated temperatures and macroscopic dimensions. This category encompasses a diverse range of systems including high-temperature superconductors, graphene, and other two-dimensional van der Waals materials, topological insulators, Dirac and Weyl semimetals, and exotic states of matter such as quantum spin liquids. A common feature among many of these materials is the critical role of reduced dimensionality, particularly the confinement of electrons to two-dimensional sheets, which dramatically enhances quantum coherence and leads to novel electronic phases that are not observed in their three-dimensional counterparts [12, 172–174].

These quantum materials form the essential building blocks for advanced quantum devices, which demand extremely precise control and manipulation of delicate quantum states. This necessity requires comprehensive investigation of their properties under extreme conditions, particularly at cryogenic temperatures where thermal fluctuations are minimized and quantum effects become dominant. The complexity of these systems has motivated the integration of artificial intelligence and machine learning methodologies into materials research. AI algorithms are now increasingly deployed to simulate intricate quantum phenomena, optimize the design and fabrication processes of qubits—the fundamental units of quantum information—and accelerate the discovery of new quantum materials with tailored properties. This includes the identification of defect-tolerant qubit architectures and the prediction of novel topological quantum spin

liquids, which are challenging to explore through traditional experimental and theoretical approaches alone [142, 175, 176].

The synergistic integration of AI with quantum computing and quantum materials science represents a highly promising and rapidly advancing frontier, poised to unlock unprecedented opportunities for scientific discovery and technological innovation. This convergence is expected to facilitate deeper insights into quantum many-body problems, enable the rational design of materials with specific quantum functionalities, and ultimately accelerate the development of practical quantum technologies [177, 178].

#### 4.8 Thermoelectric materials

Thermoelectric materials convert heat into electricity through three primary mechanisms: the Seebeck effect (generating voltage from a temperature gradient), the Peltier effect (creating a temperature gradient from electrical energy), and the Thomson effect (heat absorption or emission in a current-carrying material with a temperature difference). These phenomena are vital for sustainable energy technologies and are particularly suitable for applications in aerospace, transportation, industrial utilities, medical services, electronics, and temperature sensing [179–182].

The governing equations for these effects are:

$$\Delta V = S\Delta T, \pi_i = \frac{dQ}{dt}, \beta = \frac{|Q|}{I\Delta T} \quad (2)$$

where  $S$  is the Seebeck coefficient,  $\Delta T$  the temperature difference,  $\Delta V$  the thermoelectric voltage,  $I$  the current,  $Q$  the heat absorbed or released,  $\Pi_i$  the Peltier coefficient, and  $\beta$  the Thomson coefficient. Thermoelectric materials are classified by operating temperature: low-temperature ( $< 500$  K) thermoelectric materials such as Bismuth Chalcogenides ( $\text{Bi}_2\text{Se}_3$ ,  $\text{Bi}_2\text{Te}_3$ ,  $\text{Bi}_2\text{S}_3$ ), and Antimony Chalcogenides ( $\text{Sb}_2\text{Se}_3$ ,  $\text{Sb}_2\text{Te}_3$ ,  $\text{Sb}_2\text{S}_3$ ), the mid-temperature 500 K to 900 K thermoelectric materials like Lead Chalcogenides ( $\text{PbTe}$ ,  $\text{PbSe}$ ,  $\text{PbS}$ ), Tin Chalcogenides ( $\text{SnSe}$ ,  $\text{SnTe}$ ,  $\text{SnS}$ ), Indium Chalcogenides ( $\text{InSe}$ ,  $\text{InTe}$ ,  $\text{InS}$ ), and Germanium Chalcogenides ( $\text{GeTe}$ ,  $\text{GeSe}$ ,  $\text{GeS}$ ), and the third-class high-temperature  $> 900$  K thermoelectric materials like  $\text{SiGe}$ ,  $\text{La}_3\text{Te}_4\text{Yb}_{14}\text{MnSb}_{11}$ ,  $\text{ZrNiSn}$ , and  $\text{FeNbSb}$ -based half-Heusler alloys. [1, 182–184].

The efficiency is determined by the dimensionless figure of merit:

$$ZT = \frac{S^2 T}{\rho k} = \frac{S^2 \sigma T}{k} \quad (3)$$

where  $\sigma$  is electrical conductivity and  $\kappa$  is thermal conductivity. Enhancing  $ZT$  requires optimizing the power factor ( $S^2\sigma$ ) while minimizing  $\kappa$  through strategies like doping, band engineering, and nanostructuring to reduce.

phonon-mediated heat transport [182, 183]. Machine learning is advancing thermoelectrics across material classes. For ionic systems (i-TEs), ML navigates the complex trade-offs between ionic conductivity and stability to accelerate the discovery of novel electrolytes [185]. For electronic systems, integrated DFT-ML workflows efficiently identify high-performance semiconductors, such as predicting a high  $ZT$  in 2D tetragonal phosphorene [186].

Figure 4 demonstrates the Seebeck effect (top left) to show voltage generation ( $\Delta V$ ) from a temperature gradient ( $\Delta T$ ), enabling waste heat recovery in automotive exhaust

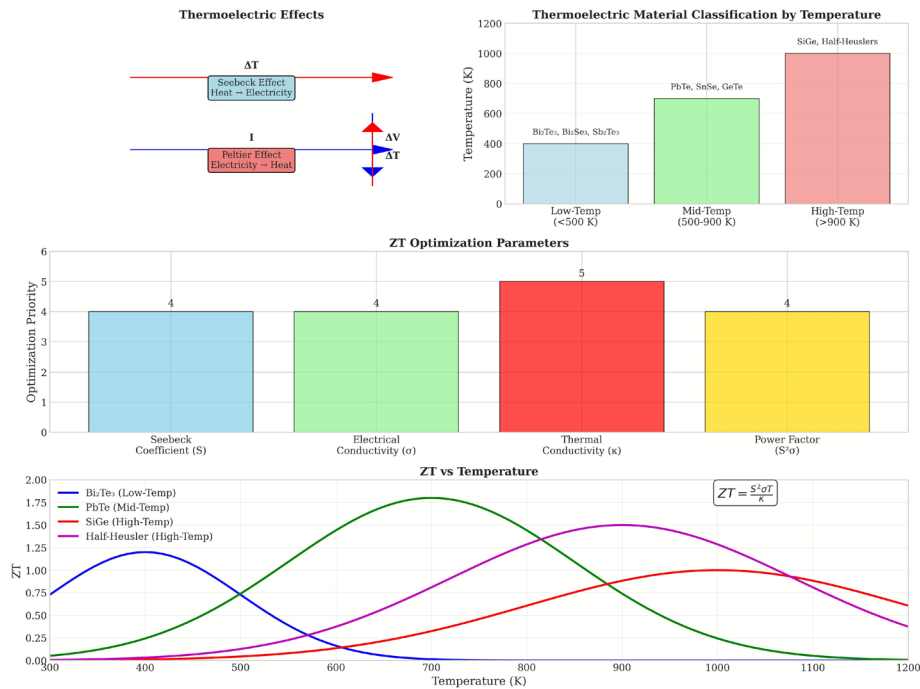


**Fig. 4** Comprehensive analysis of thermoelectric materials properties and their applications. Fundamental thermoelectric effects enabling energy conversion technologies; Material classification by operational temperature ranges; Key parameter optimization strategies for enhanced performance; Temperature-dependent efficiency characteristics guiding application-specific material selection

systems and industrial processes. The Peltier effect (bottom left) shows active cooling/heating through electrical current ( $I$ ) application, crucial for precision temperature control in medical devices, electronic cooling, and aerospace thermal management systems. The top right figure classifies thermoelectric materials by operational temperature: low-temperature materials for consumer electronics and automotive systems; mid-temperature materials for industrial waste heat recovery and solar thermal conversion; high-temperature materials for aerospace systems and high-temperature industrial processes. The middle figure shows ZT optimization priorities, with thermal conductivity reduction receiving highest priority through nanostructuring and phonon scattering, while power factor ( $S^2\sigma$ ) optimization enhances Seebeck coefficient and electrical conductivity ( $\sigma$ ) for improved energy conversion efficiency. The bottom figure displays temperature-dependent performance, with  $Bi_2Te_3$  dominating low-temperature electronic cooling, PbTe excelling in mid-temperature automotive applications, and  $SiGe$ /Half-Heuslers maintaining performance at high temperatures for space probes and industrial heat recovery.

#### 4.9 Memristors

Memristors are gaining attention for their low switching voltages, reduced power consumption, and precise gate control, enabling advancements in multiterminal memtransistors. They are a key component in neuromorphic computing and advanced electronics, exhibiting resistive switching behavior where their resistance changes based on the history of applied voltage or current. This property makes them ideal for non-volatile memory, neuromorphic applications, and energy-efficient computing [187, 188]. AI-driven methodologies have accelerated their development, optimizing material

synthesis and structural design using layered two-dimensional materials like graphene. Resistive switching mechanisms are classified into filamentary and interface-based types, with AI models predicting switching dynamics to enhance uniformity [69, 189, 190]. Memristors mimic synaptic plasticity, enabling neuromorphic systems for tasks like image recognition and spiking neural networks [191, 192]. They also perform analog logic operations within memory arrays, reducing latency and energy consumption compared to traditional architectures [193, 194].

The memristor industry is rapidly expanding, attracting significant investments and introducing advanced products to the market. This analysis examines the current state and future potential of the industry, focusing on commercially available memristor-based products, prototypes with high technological readiness, and their potential market impact. It also addresses implementation challenges and outlines pathways to overcome them. Additionally, memristors are used in true random number generators (TRNGs) for cryptographic applications due to their stochastic switching behavior, and memristive models simulate battery behavior, aiding in charge–discharge cycle analysis [195, 196].

Table 1 presents the types of electronic materials types and properties. The table systematically organizes how machine learning techniques are being deployed across diverse electronic material domains, including conductivity optimization, dielectric/magnetic material design, thermal/optical property prediction, superconductor development, traditional electronic components, ceramics/polymers, 2D materials, perovskites, quantum computing materials, catalysis, and thermoelectrics with specific AI/ML approaches.

With a comprehensive taxonomy of electronic material types and their intrinsic properties established, we proceed to explore how these materials are engineered into

**Table 1** Summary of electronic materials research categorized by key material systems and properties

| ElectronicMaterials type      | Description                                                                                                                                               | References          |
|-------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------|
| Conductive Materials          | ML models for ionic conductivity and charge transport optimization                                                                                        | [66, 68, 197]       |
| Dielectric/Magnetic Materials | AI-driven design of MXenes and magnetic materials, GANs for polymer dielectrics                                                                           | [54, 70, 175]       |
| Thermal/Optical Materials     | CNN/DL for thermal conductivity and plasmonic materials, ML for thermal transport and optoelectronic materials                                            | [74, 159, 198]      |
| Superconductor Devices        | AI for microstructure design, doping optimization, and superconductor discovery and battery cathode optimization; Sparse modeling for cuprate descriptors | [94–96, 131, 132]   |
| Resistors,Capacitors, Wires   | AI-driven synthesis of alloys and traditional components, additive manufacturing and polymer optimization                                                 | [17, 54, 79, 89]    |
| Ceramics/Polymers             | DL for bioinspired composites and crack prediction, ML for polymer composites and advanced materials design                                               | [95, 139–141]       |
| 2D Materials                  | AI virtual screening and automated characterization; GANs for graphene; transfer learning for MXenes                                                      | [59, 159, 160, 200] |
| Perovskites                   | DL for solar cell perovskites                                                                                                                             | [97]                |
| Quantum Computing             | Diffusion models for defect-tolerant qubit materials; ML for quantum materials and qubit fabrication                                                      | [12, 174–176]       |
| Catalysis                     | Neural networks for catalyst adsorption energies, AI-enhanced TEM analysis, and MXene-based catalysts                                                     | [55, 70]            |
| Thermoelectrics               | ML for high-ZT materials; Active learning for thermoelectric performance optimization                                                                     | [74, 200, 201]      |

functional devices, examining the critical relationship between material characteristics and performance across various technological domains.

## 5 Electronic materials and device applications

Revolutionary advancements in electronic materials have enabled transformative technologies including electronic chips, computers, wireless communication, and nanotechnology applications that have profoundly impacted global society through improved connectivity and miniaturized devices. Electronic materials form the foundation of modern technology, enabling applications from power conversion to neuromorphic computing. Advancements in organic composites, 2D materials, and perovskites are pushing performance boundaries, facilitating a new generation of efficient and intelligent devices [202–205]. Electronic materials are classified by their dominant charge transport and functional response, guiding their selection for devices ranging from power electronics to flexible sensors. Key classes include conductors, semiconductors, dielectrics/insulators, magnetic, and multifunctional materials, each defined by distinctive electrical, thermal, mechanical, and optical properties. The selection of a material is a complex decision based on a holistic understanding of this multifaceted profile, which enables modern technology from energy grids to biomedical devices [206–208, 243].

### 5.1 Power electronics

Electronic power devices, such as those based on 2D molybdenum disulfide ( $\text{MoS}_2$ ), are crucial for energy management in flexible systems [209]. Their switching efficiency is characterized by the on/off current ratio. The fundamental current–voltage relationship in a field-effect transistor is given by:

$$I_D = \frac{\mu C_{ox} W}{2L} (V_{GS} - V_{th})^2 \text{ for } (V_{DS} > V_{GS} - V_{th}) \quad (4)$$

where  $I_D$  is the drain current,  $\mu$  is the carrier mobility,  $C_{ox}$  is the oxide capacitance,  $W$  and  $L$  are the channel dimensions, and  $V_{GS}$  and  $V_{th}$  are the gate source and threshold voltages. These devices are essential for electric vehicles, renewable energy systems, and data centers, which require materials capable of reliable operation at high temperatures (200–400 °C) and high power. Wide-bandgap semiconductors (SiC, GaN) serve as promising alternatives to traditional Si, along with polymers for high-temperature capacitors [210–212]. Characterization under extreme conditions is critical for advancement [184, 213–215]. Artificial intelligence can transform power electronics by optimizing circuit design, predicting component failures, and enabling adaptive control strategies, leading to higher efficiency, reliability, and faster development cycles. Deep learning serves as a powerful surrogate for intensive simulations, enabling ultra-high-throughput screening. By achieving DFT-level accuracy at speeds orders of magnitude faster, these models can rapidly evaluate millions of candidate structures to identify the most promising electronic and energy materials for further investigation, drastically accelerating the discovery phase [216].

## 5.2 Optoelectronics, photonics and imaging

Optoelectronic devices convert electrical signals to optical signals. Organic cocrystals and metal halide perovskites offer tunable band gaps and high quantum efficiency [217, 218]. Photodetector performance is governed by responsivity ( $R$ ):

$$R = \frac{I_{ph}}{P_{out}} = \frac{\eta e \lambda}{hc} \quad (5)$$

where  $I_{ph}$  is the photocurrent,  $P_{opt}$  is the incident optical power,  $\eta$  is the quantum efficiency,  $e$  is the electron charge,  $\lambda$  is the wavelength,  $h$  is Planck's constant and  $c$  is the speed of light. Engineered bandgaps in compound and 2D semiconductors power LEDs, lasers, and solar devices [65, 219], while low-cost polymer-based sensors enable wide-spread applications [220, 221].

The development of solid-state electronics, initiated by the transistor, enabled reliable circuitry and integrated microprocessors that transformed computing. Subsequent nanotechnology breakthroughs yielded medical nanomaterials, while magnetic materials revolutionized diagnostic imaging through binary storage systems. Fundamental discoveries in atomic physics and electromagnetic radiation provided the foundation for medical imaging technologies, with discoveries in X-rays, radioactivity, and radium establishing essential diagnostic techniques. Photonic applications in medicine leverage lasers for precise surgical procedures, including tissue ablation, tumor removal, and vision correction. Optical fiber advances have enabled minimally invasive endoscopic procedures for gastrointestinal cancer, cardiac surgery, ulcer treatment, and lithotripsy, while laser glazing provides painless dental applications. Electromagnetic materials play a vital role in medical imaging modalities enabling disease diagnosis and therapy through interactions of electric and magnetic fields with biological systems.

The synergistic integration of magnetic and electronic materials innovation continues to drive the development of advanced medical devices with improved performance, efficiency, and sustainability, significantly advancing healthcare outcomes [222]. Through machine learning and deep learning techniques, AI enables advanced control, real-time optimization, and predictive modeling in optoelectronics, photonics, and imaging systems, accelerating innovation and performance improvements.

## 5.3 Multifunctional and sensing devices

Multifunctional devices integrate sensing, memory, and processing, and optoelectronic synapses perform mixed- color pattern recognition by responding to different light wavelengths [223]. The photoresponse is tailored using the bandgap energy:

$$E_g = \frac{hc}{\lambda_{th}} \quad (6)$$

where  $\lambda_{th}$  is the threshold wavelength. Conductive electrets [224] and ferromagnetic metal oxides [225] enable novel low-power sensors. Mixed ionic-electronic conductors, polymer-magnetic nanocomposites, and solution-processed oxides facilitate memristors, stretchable circuits, and ultrasensitive bioelectronics [65, 75, 219, 226, 227]. By integrating AI, multifunctional and sensing devices can achieve enhanced performance through predictive analysis, autonomous decision-making, and improved responsiveness.

Figure 5 describes the following main features. **FET I-V Characteristics (Power Electronics)** This plot shows the current–voltage (I–V) characteristics of a Field-Effect Transistor (FET) for different gate–source voltages ( $V_{GS} = 1.0$  V to 3.0 V). The drain current ( $I_D$ ) increases with higher  $V_{GS}$ , demonstrating the transistor's switching behavior crucial for power management in electronic circuits. The curve follows the standard MOSFET equation shown. **Photodetector Responsivity (Optoelectronics)** This figure displays how a photodetector's responsivity (electrical output per optical input) varies with the wavelength of light. The curve peaks at a specific wavelength, showing the device's optimal detection range. The responsivity is governed by the quantum efficiency ( $\eta$ ) of the material and fundamental physical constants (Planck's constant  $h$ , speed of light  $c$ , electron charge  $e$ ). **Bandgap-Wavelength Relationship** illustrates the inverse relationship between a material's bandgap energy ( $E_g$ ) and the threshold wavelength ( $\lambda_{th}$ ) of light it can absorb or emit. Wider bandgap materials respond to shorter wavelengths (bluer light), while narrower bandgaps correspond to longer wavelengths (redder light). This is fundamental for designing optoelectronic devices like LEDs and photodetectors. **Memristor Synaptic Plasticity (Neuromorphic Computing)** demonstrates how a memristor's synaptic weight ( $\Delta w$ ) changes in response to applied voltage pulses over time. This mimics neurosynaptic behavior where the "strength" of artificial synapses can be modulated, enabling brain-inspired computing and adaptive learning in neuromorphic systems. **Electronic Material Categories Comparison** A bar chart comparing the relative performance metrics of different electronic material categories (2D Materials, Perovskites, Organic Cocrystals, etc.). This visualization helps identify which material systems show the most promise for various electronic applications based on their

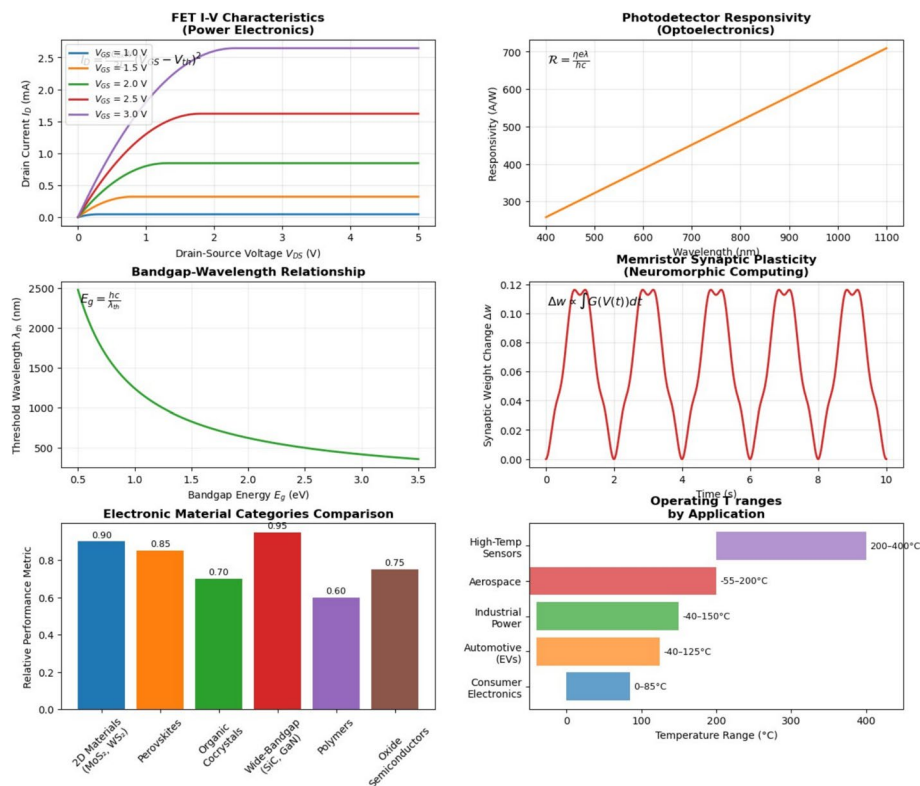


**Fig. 5** A comprehensive overview of key electronic material properties, device characteristics, and application requirements across the field of electronic materials science and engineering

quantified performance characteristics. **Operating Temperature Ranges by Application** This horizontal bar chart shows the required operating temperature ranges for electronics in different application domains. Consumer electronics have the narrowest range (0 °C to 85 °C), while high-temperature sensors must withstand the most extreme conditions (200 °C to 400 °C), highlighting the material requirements for different use cases.

#### 5.4 Memory and neuromorphic computing

Neuromorphic computing takes its cue from the human brain, designing computer systems that are not just fast but also smart and incredibly energy efficient. This approach allows machines to intuitively process sensory information like sights and sounds, learn on the fly, and tackle complex, real-world problems that baffle traditional computers. It is the key to powering a new generation of autonomous robots, advanced sensors that can see and hear with precision, seamless brain-machine interfaces, and tools that help scientists unravel the mysteries of the brain itself [228–230]. Resistive switching (RS) effects underlie nonvolatile memory and neuromorphic devices that emulate biological synapses [231]. The synaptic weight change is described by the following:

$$\Delta w \propto \int G(V(t)) dt \quad (7)$$

where  $\Delta w$  is the change in conductance and  $G(V)$  is a nonlinear function of the applied voltage. Phase-change materials, 2D TMDs like  $\text{WS}_2$ , and perovskites are widely explored for this purpose [232–235], enabling in-sensor computing that reduces power consumption and latency [236, 237]. Leveraging AI with memory-centric and neuromorphic architectures promises to accelerate learning, enhance in-sensor computation, and unlock energy-efficient, brain-inspired computing systems capable of real-time adaptation and complex decision-making.

#### 5.5 Thin-film transistors and displays

Oxide thin film transistors (TFTs) employing indium gallium zinc oxide (IGZO) semiconductors and high  $\kappa$  dielectrics such as hafnium oxide ( $\text{HfO}_2$ ) and aluminum oxide ( $\text{Al}_2\text{O}_3$ ) have significantly advanced display and large-area electronics technologies. IGZO TFTs offer high electron mobility (up to 38  $\text{cm}^2/\text{V}\cdot\text{s}$ ), low off-state leakage, and low voltage operation, making them ideal for high-resolution and flexible displays, and CMOS scaling. AI-enabled optimization of IGZO TFTs and advanced dielectrics could increase performance, flexibility, and efficiency in the next generation of displays [238, 239].

#### 5.6 Spintronics

Spintronics exploits electron spin rather than charge to develop next-generation devices. Its most significant application to date is the spin-valve magnetic sensor, which dramatically increased hard disk storage capacity. Spintronic devices offer advantages including non-volatility, low power consumption, and enhanced scalability compared to conventional electronics. These properties make them particularly promising for advanced memory-storage systems and in-memory computing applications. A notable innovation involves high-capacity solid-state memory devices that store multiple digital bits as chiral domain walls, which can be rapidly manipulated along magnetic nanowires using

**Table 2** Principal categories of electronic materials, their properties, and applications

| Material Type                                                                                        | Key Electrical Behavior                             | Applications                                         | Ref            |
|------------------------------------------------------------------------------------------------------|-----------------------------------------------------|------------------------------------------------------|----------------|
| Conductors (Cu, Al, Ag, metallic films)                                                              | High conductivity                                   | Interconnects, contacts, shielding                   | [206, 243]     |
| Semiconductors (Si, GaAs, GaN, SiC, 2DTMDs, organic variants)                                        | Tunable conductivity, bandgap control               | Transistors, LEDs, PV, detectors                     | [65, 209, 220] |
| Dielectrics/Insulators ( $\text{SiO}_2$ , $\text{HfO}_2$ , $\text{Al}_2\text{O}_3$ , ceramic oxides) | Wide bandgap, high resistivity, dielectric response | Capacitors, gate dielectrics, resonators             | [243, 244]     |
| Magnetic Materials (Ferrites, multiferroics, rare earth magnets)                                     | Spin ordering, ferro/antiferromagnetic behavior     | Memory, sensors, motors, spintronics                 | [240, 241]     |
| Piezo/Ferro-electrics (PZT, perovskite oxides)                                                       | Electric–mechanical coupling                        | Sensors, actuators, energy harvesting                | [207]          |
| Wide Bandgap & 2D Materials (SiC, GaN, graphene, MoS <sub>2</sub> , III–V/II–VI compounds)           | Large bandgaps, reduced dimensionality              | Power electronics, high-frequency devices, photonics | [75, 184]      |
| Polymers & Composites (Conductive polymers, nanocomposites, polymer-magnetic blends)                 | Tunable behavior, flexible form factors             | Wearables, flexible electronics, industrial devices  | [226, 227]     |

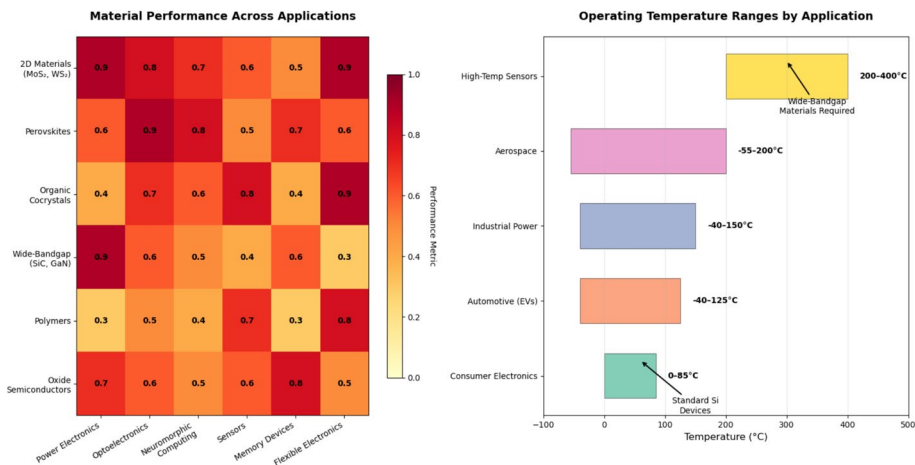


**Fig. 6** Material Performance Heatmap for electronic materials

nanosecond current pulses [240–242]. AI-driven design and control of spintronic systems can further enhance memory density, energy efficiency, and the speed of next-generation in-memory computing devices.

Table 2 describes the main classes of electronic materials based on their fundamental electrical behavior, specific material examples, which details the characteristic electrical properties that define the material category, provides representative material examples, and lists key application areas. The organization effectively shows how specific electrical behaviors enable particular applications across various technology domains.

Figure 6 contains two graphs. The first at the top left **Material Performance Heatmap** the color intensity (yellow to red) represents performance metric (0–1 scale) for six material classes across six application domains. **2D materials** excel in power electronics (0.9) and flexible electronics (0.9). **Perovskites** show peak performance in optoelectronics (0.9) and neuromorphic computing (0.8).

**Organic cocrytals** perform best in sensors (0.8) and flexible electronics (0.9). **Wide-bandgap semiconductors** dominate power electronics (0.9) but show limited flexibility.

**Polymers** excel in flexible electronics (0.8) and sensors (0.7). **Oxide semiconductors** show balanced performance with strength in memory devices (0.8). **Operating Temperature Ranges**—Colored horizontal bars show application-specific temperature requirements. **Consumer electronics** represent the baseline Si technology. **Automotive/EV applications** require extended ranges. **Industrial power**, purple) and **aerospace**, magenta) demand wider tolerances. **High-temperature sensors** require wide-band-gap materials beyond Si capabilities. The gradient from cool to warm colors visually emphasizes the increasing thermal demands in all applications.

### 5.7 Representative public datasets for AI-driven electronic materials research

The scale of materials databases has expanded dramatically, with current repositories containing vastly different amounts of data: Materials Project (154,718–170,000 materials), OQMD (1.2 million materials), and AFLOW (3.5 million materials) [245, 246]. The information in these databases has evolved from fundamental structural and thermodynamic properties to encompass complex electronic/magnetic/optical responses and electronic structures. Recent trends include incorporating symmetry information of crystals and electronic states, and expanding from perfect materials systems to heterogeneous systems such as 2D heterojunctions, surfaces, and interfaces [247].

The landscape of AI-driven electronic materials research has been fundamentally transformed by the emergence of large-scale, open-access materials databases over the past decade [247]. High-throughput computations with density-functional theory (DFT) have led to the creation of several representative databases, which have evolved from providing fundamental structural and thermodynamic properties to encompassing complex electronic, magnetic, and optical responses. These databases provide abundant, high-quality training data for artificial intelligence models, enabling unprecedented levels of generalization and improving the efficiency of materials discovery by an order of magnitude [248, 249].

Table 3 is a directory of key public datasets for AI-driven electronic materials discovery. It summarizes major repositories, listing their primary focus, key electronic properties, and applications. It includes both general-purpose databases, like Materials Project, and specialized sets for materials like perovskites. The provided properties—such as band gaps and formation energies—are essential for computational screening and machine learning, helping researchers identify data sources for predicting new functional materials.

Following a detailed analysis of the implementation of electronic materials in practical devices, we now assess the current state and future trajectory of the field. The next section addresses both the remarkable advances enabled by AI-driven approaches and the persistent challenges that must be overcome to realize the full potential of next-generation electronic materials.

## 6 Advancements, challenges and future directions in electronic materials properties and applications

The field of electronic materials is undergoing a profound and rapid evolution, driven by intensive research efforts focused on achieving higher performance metrics, introducing novel functionalities, and drastically accelerating the discovery and development process. This contemporary transformation is predominantly characterized by a strategic

**Table 3** Representative Public Datasets for AI-Driven Electronic Materials Research

| Dataset Name                          | Primary Focus                                                                                                                               | Key Electronic Properties Included                                                                                                                                          | References |
|---------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------|
| Materials Project (MP)                | DFT-calculated properties of inorganic crystalline materials; launched as part of the Materials Genome Initiative                           | Crystal structures, band gaps, formation energies, electronic structures, elastic tensors, piezoelectric properties, and various physical properties                        | [246, 250] |
| JARVIS-DFT                            | Integrated infrastructure for materials discovery using DFT, force-fields, and machine learning                                             | Formation energies, bandgaps, elastic constants, piezoelectric properties, dielectric constants, magnetic moments, Wannier tight-binding Hamiltonians, exfoliation energies | [251–253]  |
| OpenQuantum Materials Database (OQMD) | Thermodynamic and structural properties of inorganic materials from high-throughput DFT calculations                                        | Formation energies, band structures, thermodynamic stability, structural properties, electronic band gaps                                                                   | [245, 252] |
| AFLOW                                 | Comprehensive repository for inorganic crystalline materials; automated high-throughput computational framework                             | Band structures (with empirical corrections for band gaps), electronic properties, elastic tensors, thermodynamic properties                                                | [245]      |
| OMat24                                | Ultra-large dataset focused on structural and compositional diversity for inorganic bulk materials; includes non-equilibrium configurations | Formation energies, energy above hull, band gaps, density of states, elastic properties (bulk modulus, shear modulus), vibrational properties (phonon frequencies)          | [254, 255] |
| Perov-5                               | Specialized dataset for perovskite crystalline materials with compositional diversity                                                       | Crystal structures, compositional data for large perovskites with different elements                                                                                        | [250]      |
| Materialae                            | Database dedicated to topological data using structures from the Materials Project                                                          | Topological invariants, symmetry representations of occupied bands, electronic band structures for topological classification                                               | [246]      |
| Starrydata2                           | Specialized database for thermoelectric materials, digitizing graphical measurement plots from literature                                   | Thermoelectric properties (e.g., Seebeck coefficient, electrical conductivity, thermal conductivity) versus temperature                                                     | [256]      |

emphasis on precisely engineered interfaces, the development of intrinsically multifunctional materials, and a paradigm shift toward computation-assisted and data-driven discovery methodologies [238, 244, 257].

### 6.1 Notable advancements

Significant technological breakthroughs have been made in recent years. A notable advancement is the successful implementation of inorganic nanoscale semiconductors into flexible bioelectronic platforms, thereby enabling a new generation of conformable wearable health monitors and highly sensitive implantable medical sensors [226]. Currently, two-dimensional materials, including graphene and transition-metal dichalcogenides, continue to provide groundbreaking opportunities within the domain of optoelectronics, leading to the fabrication of devices exhibiting unprecedented levels of sensitivity, quantum efficiency, and operational speed [75, 219]. Furthermore, the sophisticated development of magnetoelectric heterostructures has successfully demonstrated voltage-controlled magnetism, representing a critical step towards the realization of ultra-low-power non-volatile magnetic memory and magnetologic devices [240]. The field has also witnessed the rise of innovative multifunctional composite materials that ingeniously combine distinct magnetic and semiconducting behaviors within a single material system, a development that promises to enable more highly integrated and efficient device architectures [227].

## 6.2 Key research directions

Current research is propelled by several key interdisciplinary directions. There has been an accelerated industrial adoption of wide-bandgap semiconductors, particularly silicon carbide (SiC) and gallium nitride (GaN), which are now critical for high-efficiency power conversion systems in electric vehicles and renewable energy infrastructure. This is complemented by ongoing development of novel III-V and II-VI semiconductor compounds to advance next-generation photonic devices, including micro-LED displays and high-speed radio frequency electronics [257]. A major thrust in manufacturing innovation involves the development of solution-processed metal-oxide semiconductors and dielectrics, an approach that facilitates the low-cost fabrication of large-area electronics, which is indispensable for the expansion of flexible displays, wearable sensor networks, and the ubiquitous Internet of Things (IoT) ecosystem [238]. Exploring specialized hardware for artificial intelligence, such as Neural Processing Units (NPUs), represents a promising research direction in advanced electronic materials, as these devices enable high-performance local AI computation on personal computers, reducing reliance on cloud services [258].

A significant challenge in employing two-dimensional materials has been their integration with other components; recent progress in advanced surface treatments, including hydrogenation, effectively passivates interfaces and markedly improves the performance of transistors that integrate 2D semiconductors with high- $\kappa$  dielectric materials. The paradigm of materials discovery is being revolutionized by the application of machine learning and statistical design of experiments; these powerful computational techniques are deployed to rapidly identify and optimize new material compositions, particularly in the search for novel high- $\kappa$  dielectrics for next-generation capacitors and gate oxides, thereby drastically reducing the traditional development timeline. Breaking traditional material classification boundaries, research has unveiled a new class of “polar metals” that exhibit ferroelectricity (a property typically associated with insulators) concurrently with metallicity. This unique combination of electrical polarity and conductivity opens new scientific avenues for creating electronic devices with novel switching mechanisms and non-linear optical capabilities [227, 259]. At the nanoscale, sophisticated interface engineering is being employed to tailor optical properties; techniques such as applying atomically thin graphene coatings and developing advanced dielectric models are proving effective for enhancing light reflectivity and improving electrostatic screening, which is vital for boosting the efficiency of optical devices like modulators and photodetectors.

Finally, there is growing interest in systems that exploit the complex interplay between ionic conduction and electronic transport. By meticulously engineering conductor–dielectric boundaries, researchers can modulate ionic movement to create nonvolatile memory elements (memristors) and hardware components that mimic biological neural synapses, thereby forming the foundational hardware for neuromorphic computing systems.

## 6.3 Persistent challenges

Despite the remarkable pace of progress, the application of AI in electronic materials science is a young field, and numerous fundamental methodological and theoretical problems remain open. Several formidable and interconnected challenges persist, presenting significant barriers to commercial translation and further innovation. A primary

and long-standing objective is the realization of robust and reliable room-temperature ferromagnetism in dilute magnetic semiconductors, which remains an essential prerequisite for practical and scalable spintronic applications [241]. The scalability, mechanical durability, and long-term operational reliability of flexible inorganic electronic systems also present substantial hurdles that must be conclusively overcome to ensure their commercial viability [226]. As the power density of electronic devices continues to increase, effective thermal management has emerged as a critical roadblock, particularly for high-power wide-bandgap semiconductors where heat dissipation limits performance and lifetime [260].

From a data-centric perspective, primary challenges involve the inherent scarcity and variable quality of data for novel materials, necessitating the development of standardized protocols for data curation and management [9, 261]. Furthermore, the performance and generalizability of AI models are highly dependent on the quality and diversity of training data, where biases can lead to biased predictions, and a lack of standardized benchmarking poses significant challenges to reproducibility. A critical parallel challenge lies in ensuring that AI-generated material proposals are not only theoretically optimal but also physically realistic and synthetically feasible, requiring the integration of chemical knowledge and thermodynamic constraints. Models also often suffer from performance degradation when applied outside their training domain (domain shift), highlighting the need for robust uncertainty quantification to gauge prediction reliability in novel chemical spaces. The integration of artificial intelligence with fundamental physics-based laws, while ensuring robustness and generalizability, often introduces significant computational complexity, and the substantial resources required raise concerns about environmental costs and the practical scalability of these approaches for industrial-scale materials development and qualification.

Mastering the intricate science of interface engineering is paramount for achieving strong, stable, and reliable coupling between different functional materials, such as in magnetoelectric heterostructures where the interface dictates performance [240]. Formidable hurdles remain in scaling laboratory production processes to industrial levels for promising materials like 2D heterostructures and metal halide perovskites, and in ensuring their long-term environmental stability [50]. Broader sustainability concerns encompass the environmental impact of both material synthesis and the considerable energy costs associated with large-scale AI workflows [262]. Furthermore, ethical issues, including the potential for algorithmic bias in predictive models, the existing interdisciplinary skill gaps, and the evolving intellectual property frameworks for AI-generated inventions, also pose critical challenges that the community must address [11].

Despite many advances, conventional databases face challenges with incomplete data coverage where critical material properties such as elastic moduli, thermal conductivities, or electrochemical characteristics are often missing. Discrepancies in lattice parameters or electrode potentials between different computational databases can result in unreliable data inputs. Prediction performance also varies significantly across different material properties, with properties like band gap, total energy, and formation energy achieving the lowest mean absolute error, while properties like energy above the hull and total magnetization show reduced prediction accuracy [263, 264].

#### 6.4 Future perspectives

The future trajectory of electronic materials research will be predominantly driven by the deepening integration of artificial intelligence, shows promise in bridging the historical gap between computation and experiment in specific workflows (e.g., high-throughput DFT guiding synthesis), though significant challenges in data integration and transferability remain [265–267]. Critical future frontiers on this horizon include the widespread adoption and standardization of self-driving labs (SDLs) for autonomous experimentation [268], the development and deployment of large-scale, general-purpose foundation models specifically tailored for materials science [269], and the dedicated application of AI for the design and optimization of quantum computing hardware components [270]. Advancing the field of explainable AI (XAI) to demystify the decision-making processes of complex models will be crucial for building trust and extracting fundamental scientific insights [13]. Scaling emerging neuromorphic computing.

platforms based on novel materials and device concepts will be essential for implementing next-generation artificial intelligence hardware [271]. Finally, promoting global open data initiatives within robust, equitable, and transparent ethical frameworks will be indispensable for fostering sustainable, collaborative, and innovative growth across the entire field [272]. Moving beyond performance, the next frontier for generative AI in materials is interpretability. Interpretable surrogate frameworks can distill a neural network's complex decisions into human-understandable design rules. This reveals the fundamental structural or compositional descriptors behind optimal properties, providing crucial scientific insight, building trust in AI-generated candidates, and guiding further human exploration [273].

The transformative impact of AI and machine learning on materials discovery is manifested in their ability to enable the rapid prediction of complex properties, the optimization of synthesis and processing pathways, and the generative design of novel compounds with targeted functionalities. Sophisticated algorithms are now capable of analyzing vast, multi-modal datasets to accurately predict key electronic properties such as thermal conductivity and band structure, particularly in complex low-dimensional systems like 2D transition metal dichalcogenides. Generative models, including polyG2G, are significantly accelerating the rational design of polymers and organic electronic materials, while active learning and diffusion models efficiently navigate the vast compositional space of inorganic materials to propose promising candidates with targeted electronic functionalities [12, 54, 274].

Underpinning this progress are significant computational advances. Deep learning models are increasingly used to predict electronic structures directly, and transfer learning techniques leverage insights gained from one material class to accelerate discovery in another. Comprehensive computational frameworks such as the Joint Automated Repository for Various Integrated Simulations (JARVIS) and the Scientific Machine Intelligence Learning Education (SMILE) platform integrate massive computed databases to streamline and automate property prediction [56, 275]. Furthermore, autonomous laboratories are beginning to automate synthesis and characterization, thereby creating closed-loop, high-throughput discovery systems that can operate with minimal human intervention [49]. AI also optimizes complex analytical workflows, such as the analysis of transmission electron microscopy (TEM) data, and effectively mitigates data scarcity through sophisticated active learning and data augmentation strategies [55, 276].

A key conceptual innovation is the use of AI to finally bridge the historical gap between computation and experiment. AI-driven multi-fidelity models integrate data from high-throughput DFT simulations and a wide array of experimental characterization techniques — including electrical (IV, CV, Hall effect, DLTS), structural (XRD, SEM/TEM), optical (photoluminescence, Raman), and chemical (EDX, XPS) analyses — to create a collaborative and iterative framework. This synergy creates a powerful feedback loop that continuously refines predictions in real time, overcoming the limitations of traditional trial-and-error approaches and the high computational cost and functional-dependent inaccuracies often associated with standalone DFT calculations [277].

Specific AI architectures are now driving tangible breakthroughs. Physics-informed neural networks (PINNs) seamlessly embed quantum mechanical constraints and governing equations to resolve multiscale electronic behaviors with high fidelity [80, 278]. Generative adversarial networks (GANs) are being employed for the inverse design of novel perovskite compositions with targeted bandgaps for photovoltaics and optoelectronics [146]. Reinforcement learning agents optimize complex synthesis parameters for advanced materials like high-entropy alloys, drastically reducing the number of required experimental iterations [279]. Explainable AI methods are crucial for clarifying the relationship between material features (e.g., crystal structure, defects) and resulting electronic properties, while Bayesian deep learning provides a robust probabilistic framework for uncertainty-aware inverse design [13]. This integrated, AI-driven paradigm is fundamentally accelerating the development cycle of next-generation electronic materials for transformative applications in flexible electronics, advanced energy storage systems, and scalable quantum computing [280].

## 7 Conclusion

Based on a comprehensive review of the field, this paper concludes that the landscape of electronic materials research is undergoing a profound transformation, driven by the synergistic integration of artificial intelligence and machine learning with foundational materials science principles. The critical analysis of material properties—spanning conductors, semiconductors, dielectrics, 2D materials, perovskites, quantum materials, and more—reveals that AI-driven methodologies are not merely incremental tools but are enabling a paradigm shift from traditional trial-and-error approaches to accelerated, predictive, and generative design. Techniques such as Physics-Informed Neural Networks, Generative Adversarial Networks, Graph Neural Networks, and Reinforcement Learning are demonstrating significant potential in bridging the gap between quantum-level behavior and macroscopic properties, optimizing multifunctional performance, and enabling inverse design.

Despite these advancements, persistent challenges remain, including data scarcity, model interpretability, thermal management, scalability, and the integration of multidisciplinary datasets. Future progress hinges on addressing these issues through the development of explainable AI, robust foundation models, self-driving laboratories, and standardized open-data initiatives. The continued convergence of computational prediction, AI-driven discovery, and experimental validation holds the promise of unlocking next-generation electronic materials tailored for transformative applications in power electronics, neuromorphic computing, quantum technologies, and sustainable energy systems. Ultimately, this integrated, intelligent framework is poised to revolutionize the

entire materials development lifecycle, fostering a new era of innovation and efficiency in electronic materials science and engineering.

#### Author's contributions

The authors have contributed from the start of conceptualization, writing, editing, compiling, and submission of the paper. Wubshet Getachew Mengesha conceptualized the paper, prepared tables and figures, supervised the timelines, wrote the original draft, reviewed and edited, and submitted the final work. Kaveer Nagessar drafted the manuscript, prepared equations, tables, and figures, and critically reviewed and edited the manuscript. Both authors collaboratively refined the article with iterative discussions and jointly revised the final version to ensure logical coherence, technical accuracy, and alignment with publication standards.

#### Funding

The paper was conducted in the absence of any financial aid.

#### Data availability

No datasets were generated or analysed during the current study.

#### Declarations

##### Ethical approval and consent to participate

Not applicable.

##### Consent for publication

Not applicable.

##### Competing interests

The authors declare no competing interests.

Received: 11 September 2025 / Accepted: 19 December 2025

Published online: 26 December 2025

#### References

1. Schafrik RE, Walston S, "Challenges for high temperature materials in the new millennium," 2008; [https://doi.org/10.7449/2008/SUPERALLOYS\\_2008\\_3\\_9](https://doi.org/10.7449/2008/SUPERALLOYS_2008_3_9)
2. Pint BA. Critical assessment 4: challenges in developing high temperature materials. *Mater Sci Technol*. 2014;30(12):1387–91. <https://doi.org/10.1179/1743284714Y0000000580>.
3. Adetunla A, Akinlabi E, Jen TC, Ajibade S-S, "Harnessing the power of artificial intelligence in materials science: An overview," in *2024 Intern. Confe.Sci., Engin. Busi. Driv. Sustai. Develop. Goals (SEB4SDG)*, 2024; <https://doi.org/10.1109/SEB4SDG60871.2024.10630185>
4. Carmo LHD, et al. Electrochemical preparation of polymers for energy storage. *Prog Polym Sci*. 2023. <https://doi.org/10.102/prep.202200276>.
5. Li B, Gilbert S. Artificial intelligence awarded two nobel prizes for innovations that will shape the future of medicine. *NPJ Digit Med*. 2024;7:336. <https://doi.org/10.1038/s41746-024-01345-9>.
6. Pasupuleti MK, "AI-powered materials innovation: Accelerating design and discovery in advanced materials," *NESX – Internat. J. Academ. Indus. R. Innovat.*, 2024; <https://doi.org/10.62311/nexx/46618>
7. Schmidt J, et al. Machine learning in materials science. *Adv Mater*. 2019;31(22):1901130. <https://doi.org/10.1002/adma.201901130>.
8. Curtarolo S, et al. The high-throughput highway to computational materials design. *Nat Mater*. 2013;12(11):1005–15. <https://doi.org/10.1038/nmat3768>.
9. Merchant A, Batzner S, Schoenholz S, Aykol M, Cheon G, Cubuk ED. Scaling deep learning for materials discovery. *Nature*. 2023;624:80–5. <https://doi.org/10.1038/s41586-023-06735-9>.
10. Choudhary K, et al. Hybrid computational-experimental workflows for accelerated materials discovery. *Nat Rev Mater*. 2022;7(7):564–85. <https://doi.org/10.1038/s41578-022-00439-1>.
11. Jha D, Ward L, Choudhary A, Wolverton C. Elemnet: Deep learning the chemistry of materials from the periodic table. *Sci Rep*. 2018. <https://doi.org/10.1038/s41598-018-35816-5>.
12. Ni B, Kaplan DL, Buehler MJ. Generative design of de novo proteins based on secondary-structure constraints using an attention-based diffusion model. *Chem*. 2023;9:1828–49. <https://doi.org/10.1016/j.chempr.2023.03.020>.
13. Qayyum F, Alil M, Kim D, Ko H-S, Ryu G-A. Explainable AI for material property prediction based on energy cloud: a Shapley-driven approach. *Materials*. 2023;16(23):7322. <https://doi.org/10.3390/ma16237322>.
14. Kulik H, et al. Roadmap on machine learning in electronic structure. *Electronic Structure*. 2022. <https://doi.org/10.1088/2516-1075/ac572f>.
15. Lauw L, Baker N, Nguyen DT, Mueller KT, Lee SJ, Chen C, et al. Accelerating computational materials discovery with machine learning and cloud high-performance computing: from large-scale screening to experimental validation. *J Am Chem Soc*. 2024. <https://doi.org/10.1021/jacs.4c03849>.
16. Xu Y, Wang Q, An Z, Wang F, Zhang L, Wu Y, et al. Artificial intelligence: a powerful paradigm for scientific research. *The Innovation*. 2021. <https://doi.org/10.1016/j.xinn.2021.100179>.
17. Pyzer-Knapp EO, Pitera J, Staar P, Takeda S, Laino T, Sanders DP, et al. Accelerating materials discovery using artificial intelligence, high performance computing and robotics. *NPJ Comput Mater*. 2022;8:1–9. <https://doi.org/10.1038/s41524-022-00765-z>.

18. Morgan D, Jacobs R. Opportunities and challenges for machine learning in materials science. *Annu Rev Mater Res*. 2020. <https://doi.org/10.1146/annurev-matsci-070218-010015>.
19. Dan Y, Zhao Y, Li X, Li S, Hu M, Hu J, "Generative adversarial networks (gan) based efficient sampling of chemical composition space for inverse design of inorganic materials," *npj Computational Materials*, 2019; <https://doi.org/10.1038/s41524-020-00352-0>
20. Zhao Y, Al-fahdi M, Hu M, Siriwardane E, Song Y, Nasiri A, et al. High-throughput discovery of novel cubic crystal materials using deep generative neural networks. *Adv Sci*. 2021. <https://doi.org/10.1002/adv.202100566>.
21. Rashid MM, Chakraborty S, Krishnan N. Revealing the predictive power of neural operators for strain evolution in digital composites. *J Mech Phys Solids*. 2023. <https://doi.org/10.1016/j.jmps.2023.105444>.
22. Lee J, Su H. Rethinking industrial artificial intelligence: a unified foundation framework. *International Journal of AI for Materials and Design*. 2025. <https://doi.org/10.36922/IJAMD025080006>.
23. Abdelraouf OAM, Ahmed AMA, Eldele E, Omar AA, "Physics-informed neural networks in electromagnetic and nanophotonic design," 2025
24. Patel KP, Maicke A, Arzate J, Kwon J, Smith JD, Aimone J, Incorvia J, Cardwell S, Schuman CD, "Ai-guided codesign framework for novel material and device design applied to mtj-based true random number generators," *arXiv.org*, 2024; <https://doi.org/10.48550/arXiv.2411.01008>
25. Regenwetter L, Nobari A, Ahmed F. Deep generative models in engineering design: A review. *J Mech Des*. 2021. <https://doi.org/10.1115/1.4053859>.
26. Sanchez-Lengeling B, Aspuru-Guzik A. Inverse molecular design using machine learning: Generative models for matter engineering. *Science*. 2018. <https://doi.org/10.1126/science.aat2663>.
27. So S, Rho J. Designing nanophotonic structures using conditional deep convolutional generative adversarial networks. *Nanophotonics*. 2019. <https://doi.org/10.1515/nanoph-2019-0117>.
28. Mao Y, He Q, Zhao X. Designing complex architected materials with generative adversarial networks. *Sci Adv*. 2020. <https://doi.org/10.1126/sciadv.aaz4169>.
29. Yang Y, Liu Y, Wu Z, Zhang Y, Wang W, Hou Y, Zhang Y, He J, Wang L, Liu X. *et al.*, "Selective hydrogenation improves interface properties of high-k dielectrics on 2d semiconductors," *arXiv preprint*, 2021. <http://arxiv.org/abs/2110.06586>
30. Martin TB, Audus DJ. Emerging trends in machine learning: a polymer perspective. *ACS Polym Au*. 2023. <https://doi.org/10.1021/acspolymersau.2c00053>.
31. Aldeghi M, Coley CW. A graph representation of molecular ensembles for polymer property prediction. *Chem Sci*. 2022. <https://doi.org/10.1039/D2SC02839E>.
32. Xie T, Grossman J. Crystal graph convolutional neural networks for an accurate and interpretable prediction of material properties. *Phys Rev Lett*. 2017. <https://doi.org/10.1103/PhysRevLett.120.145301>.
33. Choudhary K, DeCost B L, "Atomistic line graph neural network for improved materials property predictions," *npj Computational Materials*, 2021. s41524–021–00650–1
34. Liu J, Tang Y, Tretiak S, Duan W, Zhou L, "Sa-gat-sr: Self-adaptable graph attention networks with symbolic regression for high-fidelity material property prediction," *arXiv.org*, 2025; <https://doi.org/10.48550/arXiv.2505.00625>
35. Witman M, Goyal A, Ogitsu T, McDaniel A, Lany S. Defect graph neural networks for materials discovery in high-temperature clean-energy applications. *Nat Comput Sci*. 2023. <https://doi.org/10.1038/s43588-023-00495-2>.
36. Arulkumar K, Deisenroth M, Brundage M, Bharath A. Deep reinforcement learning: a brief survey. *IEEE Signal Process Mag*. 2017. <https://doi.org/10.1109/MSP.2017.2743240>.
37. Cho S-H, Kim Y-S. An overview of artificial intelligence and machine learning in shoulder surgery. *Clin Shoulder Elbow*. 2025. <https://doi.org/10.5397/cise.2025.00185>.
38. Ma T, Chakraborty P, Guo X, Cao L, Wang Y. First-principles modeling of thermal transport in materials: achievements, opportunities, and challenges. *Int J Thermophys*. 2020;41(1):1–37. <https://doi.org/10.1007/S10765-019-2583-4>.
39. Nene P, Thankachan D. Design of an intelligent ai-based multi-layer optimization framework for grid-tied solar pv-fuel cell hybrid energy systems. *MethodsX*. 2025. <https://doi.org/10.1016/j.mex.2025.103540>.
40. Handoko A D, Made RI, "Artificial intelligence and generative models for materials discovery – a review," 2025. <https://api.semanticscholar.org/CorpusID:280527170>
41. Zhang B, Li X, Xu H, Jin Z, Wu Q, Li C, "Topomas: Large language model driven topological materials multiagent system," *arXiv.org*, 2025; <https://doi.org/10.48550/arXiv.2507.04053>
42. Ma X, Lewis JP, Yan Q-B, Su G. Accelerated discovery of two-dimensional optoelectronic octahedral oxyhalides via high-throughput *ab initio* calculations and machine learning. *J Phys Chem Lett*. 2019. <https://doi.org/10.1021/acs.jpclett.9b02420>.
43. Lu S, Zhou Q, Ouyang Y, Guo Y, Li Q, Wang J. Accelerated discovery of stable lead-free hybrid organic-inorganic perovskites via machine learning. *Nat Commun*. 2018. <https://doi.org/10.1038/s41467-018-05761-w>.
44. Ottomano F, "Assessing data-driven predictions of band gap and electrical conductivity for transparent conducting materials," *arXiv.org*, 2024; <https://doi.org/10.48550/arXiv.2411.14034>
45. Montavon G, Rupp M, Gobre VV, Zquez-Mayagoitia Va, Hansen K, Tkatchenko A, Tkatchenko A, Müller K, Müller K-R, Lilienfeld OV, "Machine learning of molecular electronic properties in chemical compound space," 2013; <https://doi.org/10.1088/1367-2630/15/9/095003>
46. Selvaraj SC, "Graph neural networks based deep learning for predicting structural and electronic properties," 2024. <https://api.semanticscholar.org/CorpusID:273821595>
47. Nematov D, Hojamberdiev M. Machine learning-driven materials discovery: unlocking next-generation functional materials – a review. *Comput Condens Matter*. 2025. <https://doi.org/10.1016/j.cocom.2025.e01139>.
48. Ninduwzeor-Ehiobu N, Alaba O, Daraojimba C, Ofonagoro KA, Ogunjobi OA, Gidiagba JO, et al. "Tracing the evolution of ai and machine learning applications in advancing materials discovery and production processes," *Engineering Science and Technology Journal*. 2023. <https://doi.org/10.51594/estj.v4i3.552>.
49. Han X-Q, Wang X-D, Xu M-Y, Feng Z, Yao B-W, Guo P-J, Gao Z-F, Lu Z-Y, "Ai-driven inverse design of materials: Past, present and future," *arXiv*, vol. abs/2411.09429, 2024. <https://api.semanticscholar.org/CorpusID:274023350>
50. Soldatov M, Butova V, Pashkov D, Butakova M, Medvedev P, Chernov A, et al. Self-driving laboratories for development of new functional materials and optimizing known reactions. *Nanomaterials*. 2021. <https://doi.org/10.3390/nano11030619>.

51. Qiao H, Liu H, Huang Z, Hu R, Ma Q, Zhong J, et al. Tunable electronic and optical properties of 2d monoelemental materials beyond graphene for promising applications. *Energy Environmental Materials*. 2020. <https://doi.org/10.1002/eem.12154>.
52. Song Y, Miret S, Zhang H, Liu B, "Honeybee: Progressive instruction finetuning of large language models for materials science," in *Conference on Empirical Methods in Natural Language Processing*, 2023. <https://api.semanticscholar.org/CorpusId:263909166>
53. Zhang H, Zhang X, Pan D, Ai Y, Chen YW. Preparation and application of high-temperature composite phase change materials. *J Energy Storage*. 2023;68:107669. <https://doi.org/10.1016/j.est.2023.107669>.
54. Gurnani R, Kamal D, Tran H, Sahu H, Scharm K, Ashraf U, et al. Polyg2g: a novel machine learning algorithm applied to the generative design of polymer dielectrics. *Chem Mater*. 2021;33:7008–16. <https://doi.org/10.1021/acs.chemmater.1c02061>.
55. A. Cabot, E. Rotunno, T. Galvani, G. Katsaros, P. Krogstrup, J. Arbiol, M. C. Spadaro, G. Scappucci, M. B. Eriksen, I. Pinto-Huguet, G. Isella, M. Botifoll, Y.-M. Niquet, S. Mart'i-S'anchez, S. Roche, V. Grillo, P. Ordej'ón, P. H. Kavkani, C. Coll, and G. Merino, "Artificial intelligence end-to-end workflow for transmission electron microscopy: From data analysis automation to materials knowledge unveiling," 2024. <https://api.semanticscholar.org/CorpusId:273811319>
56. Biacchi AJ, DeCost BL, Wines D, Gurunathan R, Garrity KF, Choudhary K, et al. Recent progress in the jarvis infrastructure for next-generation data-driven materials design. *Appl Phys Rev*. 2023. <https://doi.org/10.1063/5.0159299>.
57. Tagade PM, Adiga SP, Pandian S, Park MS, Hariharan KS, Kolake SM. Attribute driven inverse materials design using deep learning bayesian framework. *NPJ Comput Mater*. 2019;5:127. <https://doi.org/10.1038/s41524-019-0263-3>.
58. Tsao J, Chowdhury S, Hollis M, Jena D, Johnson N, Jones K, Kaplar R, Rajan S, Walle C D, Bellotti E, Chua C, Collazo R, Coltrin M, Cooper J, Evans K, Graham S, Grotjohn T, Heller E, Higashiwaki M, Islam M, Juodawlkis P, Khan M A, Koehler A, Leach J, Mishra U, Nemanich R, Pilawa-Podgurski R, Shealy J, Sitar Z, Tadjer M, Witulski A, Wraback M, Simmons J, "Ultrawide-band-gap semiconductors: Research opportunities and challenges," *Advanced Electronic Materials*, vol. 4, 2018. <https://api.semanticscholar.org/CorpusId:38628999>
59. Jiang M, Huang Z, Qiu L, Huang W, Yen GG. Transfer learning-based dynamic multiobjective optimization algorithms. *IEEE Trans Evol Comput*. 2018;22:501–14. <https://doi.org/10.1109/TEVC.2017.2771451>.
60. Guo C, Tan Y, Zhu J, Xie J, Gu C, Hu W. High quality cuinp2s6 single crystal for intrinsic electric property. *J Materiomics*. 2025. <https://doi.org/10.1016/j.jmat.2025.101067>.
61. D. B. Straus and C. Kagan, "Photophysics of two-dimensional semiconducting organic-inorganic metal-halide perovskites." *Annual rev. phy. chemi*. 2021: <https://api.semanticscholar.org/CorpusId:237363938>
62. Zhang L, "Advances in the application of perovskite materials," *Nano-Micro Letter*, 2023. 15, <https://api.semanticscholar.org/CorpusId:259377397>
63. Li H, Xu X. Electronic structures of ge2sb2te5/co2fex (x: Al, si) interfaces for phase change spintronics. *ACS Omega*. 2018. <https://doi.org/10.1021/ACSOMEGA.8B02016>.
64. Wang G, Tang Z, Gao Y, Liu P, Li Y, Li A, et al. Phase change thermal storage materials for interdisciplinary applications. *Chem Rev*. 2023;123(11):6953–7024.
65. Nogueira AE, Ribeiro LS, Nogueira FGE, Torres JA. "Semiconductors", in *Advanced Materials for Sustainable Energy and Engineering*. CRC Press. 2024. <https://doi.org/10.1201/9781003450146-1>.
66. Ahmad Z, Xie T, Maheshwari C, Grossman J, Viswanathan V. Machine learning enabled computational screening of inorganic solid electrolytes for suppression of dendrite formation in lithium metal anodes. *ACS Cent Sci*. 2018;4:996–1006.
67. Wang QH, Kalantar-zadeh K, Kis A, Coleman J, Strano M. Electronics and optoelectronics of two-dimensional transition metal dichalcogenides. *Nat Nanotechnol*. 2012;7(11):699–712.
68. Deng B, Zhong P, Jun K, Riebesell J, Han K, Bartel CJ, et al. Chgnet as a pretrained universal neural network potential for charge-informed atomistic modelling. *Nat Mach Intell*. 2023;5:1031–41. <https://doi.org/10.1038/s42256-023-00716-3>.
69. Wang M, Cai S, Pan C, Wang C-Y, Lian X, Xu K, et al. Robust memristors based on layered two-dimensional materials. *Nat Electron*. 2018;1:130–6. <https://doi.org/10.1038/s41928-018-0021-4>.
70. Iravani S, Khosravi A, Zare EN, Varma RS, Zarrabi A, Makvandi P. Mxenes and artificial intelligence: fostering advancements in synthesis techniques and breakthroughs in applications. *RSC Adv*. 2024;14:36 835.
71. Jiles D, Kiarie W. An integrated model of magnetic hysteresis, the magnetomechanical effect, and the barkhausen effect. *IEEE Trans Magn*. 2021;57(2):1–11. <https://doi.org/10.1109/TMAG.2020.3034208>.
72. Li D, Gong Y, Chen Y, Lin J-H, Khan Q, Zhang Y, et al. Recent progress of two-dimensional thermoelectric materials. *Nano-Micro Lett*. 2020. <https://doi.org/10.1007/s40820-020-0374-x>.
73. Huo B, Guo C. Advances in thermoelectric composites consisting of conductive polymers and fillers with different architectures. *Molecules*. 2022;3:252983064.
74. Hu M, "Unleashing the power of artificial intelligence in phonon thermal transport: Current challenges and prospects," *J. Applied Phy*. 2024, <https://api.semanticscholar.org/CorpusId: 269655943>
75. Suresh S, "Semiconductor nanomaterials, methods and applications: A review," *Nanoscience and Nanotechnology*, 2013; 3, 3, 62–74, [https://www.sciencepub.net/nanotech/ nanotech0303/10\\_017\\_0303\\_nanotech\\_62\\_74.pdf](https://www.sciencepub.net/nanotech/ nanotech0303/10_017_0303_nanotech_62_74.pdf)
76. Braun D, Ganeriwala M D, Volkel L, Ran K, Lukas S, Mar'in E G, Hartwig O, Prechtl M, Wahlbrink T, Mayer J, Duesberg G, Godoy A, Daus A, Lemme M, "Non-volatile resistive switching of polymer residues in 2d material memristors," in *unknown*, 2023. <https://api.semanticscholar.org/CorpusId:262465193>
77. EE Power, "Basic principles of power electronics.": <https://eepower.com/resistor-guide/>
78. Miller LS, Mullin JB, Eds, *Electronic Materials: From Silicon to Organics*, 1st ed., ser. Springer Book Archive. New York, NY: Springer New York, 1991 <https://doi.org/10.1007/978-1-4615-3818-9>
79. Badini S, Regondi S, Frontoni E, Pugliese R. Assessing the capabilities of ChatGPT to improve additive manufacturing troubleshooting. *Adv Ind Eng Polym Res*. 2023;6:278–87. <https://doi.org/10.1016/j.aiepr.2023.03.003>.
80. Jeong I, Cho M, Chung H, Kim D-N. Data-driven nonparametric identification of material behavior based on physics-informed neural network with full-field data. *Comput Methods Appl Mech Eng*. 2024. <https://doi.org/10.1016/j.cma.2023.116569>.
81. Habib M, Farhad S, Tanvir N, Alam M, Bitu M, Islam M S, Islam S, Khatun N, Hossain M S, "Fabrication and characterization of graphene-barium titanate-graphene layered capacitors by spin coating at low processing temperatures," *ECS J. Solid State Sci. Techno*. 2023. <https://api.semanticscholar.org/CorpusId:259202726>

82. Reenu, Sonia, Phor L, Kumar A, Chahal S, "Electrode materials for supercapacitors: A comprehensive review of advancements and performance," *J. Ene. Storage*, 2024; 84. 110698: <https://www.sciencedirect.com/science/article/pii/S2352152X24002822>
83. Yaseen M, Khattak M A K, Humayun M, Usman M, Shah S S, Bibi S, Hasnain B S U, Ahmad S M, Khan A, Shah N, Tahir A A, Ullah H, "A review of supercapacitors: Materials design, modification, and applications," *Ener.*, 2021; 14. 22, <https://www.mdpi.com/1996-1073/14/22/7779>
84. Manyala N, Thior S, Kitege VN, Diop NF, Otun K, Maphiri V, et al. Enhancing potential window with ionic liquid/water in salt mixture in co-doped activated carbon electrodes for high-energy supercapacitors. *SSRN Electron J.* 2024. <https://doi.org/10.2139/ssrn.5383614>.
85. Hashim A. Enhanced structural, optical, and electronic properties of  $\text{In}_2\text{O}_3$  and  $\text{Cr}_2\text{O}_3$  nanoparticles doped polymer blend for flexible electronics and potential applications. *J Inorg Organomet Polym Mater.* 2020;30:3894–906. <https://doi.org/10.1007/s10904-020-01528-3>.
86. Tiwari A, Bansal G, Mukhopadhyay SJ, Bhattacharjee A, Kanungo S. Quantum capacitance engineering in boron and carbon modified monolayer phosphorene electrodes for supercapacitor application: a theoretical approach using ab-initio calculation. *J Energy Storage.* 2023;73:109040.
87. Zhou X, Wang Y, "Ab initio simulation and analysis of the charge couples in rechargeable batteries and supercapacitors," *ECS Meet Abst.*, 2017; 22. 1148, <https://doi.org/10.1149/MA2017-01/22/1148>
88. Mishra N, Bahadursha N, Reddy AS, Kanungo S, Bhattacharjee A. Ab-initio calculation driven machine learning based prediction of quantum capacitance of titanium-doped graphene for efficient supercapacitor electrode design. *J Energy Storage.* 2025;107:115038.
89. Ghafarollahi A, Buehler MJ. Automating alloy design and discovery with physics-aware multimodal multiagent ai. *Proc Natl Acad Sci U S A.* 2025;122(4):e2414074122.
90. Vandenberghe WG. Determining electronic, structural, dielectric, magnetic, and transport properties in novel electronic materials: using first-principles techniques. *IEEE Nanotechnol Mag.* 2021. <https://doi.org/10.1109/MNANO.2021.3113223>.
91. Xu J, Luo Z, Chen L, Zhou X, Zhang H, Zheng Y, et al. Recent advances in flexible memristors for advanced computing and sensing. *Mater Horiz.* 2024. <https://doi.org/10.1039/D4MH00291A>.
92. Zhou H, et al. Machine learning-guided fabrication of high-performance transistors. *Sci Adv.* 2023. <https://doi.org/10.1126/sciadv.adg2023>.
93. Li X, et al. Deep learning for exfoliation energy prediction in layered compounds. *Nat Commun.* 2023. <https://doi.org/10.1038/s41467-023-38910-z>.
94. Chun S, Roy S, Nguyen YT, Choi JB, Udaykumar HS, Baek SS. Deep learning for synthetic microstructure generation in a materials-by-design framework for heterogeneous energetic materials. *Sci Rep.* 2020;10:13307. <https://doi.org/10.1038/s41598-020-70149-0>.
95. Shen SCY, Fernandez MP, Tozzi G, Buehler MJ. Deep learning approach to assess damage mechanics of bone tissue. *J Mech Behav Biomed Mater.* 2021;123:104761. <https://doi.org/10.1016/j.jmbbm.2021.104761>.
96. Ceder G, Lun Z, Zhong P, He T, Deng B, "Deep learning of experimental electrochemistry for battery cathodes across diverse compositions," *Joule*, 2023. <https://api.semanticscholar.org/CorpusId:258059749>
97. Zhang J, Hauch J, Brabec CJ. Toward self-driven autonomous material and device acceleration platforms (amadap) for emerging photovoltaics technologies. *Acc Chem Res.* 2024;57:1434–45.
98. Noe P, Vallée C, Hippert F, Fillot F, Raty J-Y. Phase change materials for non-volatile memory devices: from technological challenges to materials science issues. *Semicond Sci Technol.* 2018;33(1):013002. <https://doi.org/10.1088/1361-6641/AA7C25>.
99. Liu J, Long Y, Bai D, Sun H, Zhang H, Kewen L, et al. Magnetic properties of feni alloys for high-temperature thermomagnetic power generation. *AIP Adv.* 2019;9(4):045227. <https://doi.org/10.1063/1.5086411>.
100. Zhang W, Mazzarello R, Ma E. Phase-change materials in electronics and photonics. *MRS Bull.* 2019;44(9):686–90. <https://doi.org/10.1557/mrs.2019.201>.
101. Roknuzzaman M, Zhang C, Ostrikov K, Du A, Wang H, Wang L, et al. Electronic and optical properties of lead-free hybrid double perovskites for photovoltaic and optoelectronic applications. *Sci Rep.* 2019. <https://doi.org/10.1038/s41598-018-37132-2>.
102. Khazaei M, Ranjbar A, Arai M, Sasaki T, Yunoki S, "Electronic properties and applications of mxenes: a theoretical review," *Journal of Materials Chemistry C*, vol. 5, pp. 2488–2503, 2017. [Online]. Available: <https://arxiv.org/pdf/1702.07442.pdf>
103. Tilli M, Haapalinna A, "Chapter 1 - properties of silicon," in *Handbook of Silicon Based MEMS Materials and Technologies (Third Edition)*, 3rd ed., ser. Micro and Nano Technologies, M Tilli, M Paulasto-Krockel, M Petzold, H Theuss, T Motooka, V Lindroos, Eds. Elsevier, 2020; <https://doi.org/10.1016/B978-0-12-817786-0.00001-3>
104. Varshni Y. Temperature dependence of the energy gap in semiconductors. *Physica.* 1967;34(1):149–54.
105. Kuwata-Gonokami M, "High-density excitons in semiconductors," in *Refe. Mod.Mate. Sci. Mat. Eng.*. Elsevier, 2016. <https://www.sciencedirect.com/science/article/pii/B9780128035818007815>
106. Barron A, *Chemistry of the Main Group Elements*. Rice University via CNX, 2024: [https://chem.libretexts.org/Bookshelves/Inorganic\\_Chemistry/Chemistry\\_of\\_the\\_Main\\_Group\\_Elements\\_\(Barron\)](https://chem.libretexts.org/Bookshelves/Inorganic_Chemistry/Chemistry_of_the_Main_Group_Elements_(Barron))
107. Lindsay L, "2 - first principles thermal transport modeling in gan and related materials\*", in *Thermal Management of Gallium Nitride Electronics*, ser. Woodhead Publishing Series in Electronic and Optical Materials, M. J. Tadjer and T. J. Anderson, Eds. Woodhead Publishing, 2022, pp. 21–43. <https://www.sciencedirect.com/science/article/pii/B9780128210840000160>
108. Porter L, Das K, Dong Y, Melby J, Virshup A, "Contacts to wide-band-gap semiconductors," in *Comprehensive Semiconductor Science and Technology*, P. Bhattacharya, R. Fornari, and H. Kamimura, Eds. Amsterdam: Elsevier, 2011; 44–85. <https://www.sciencedirect.com/science/article/pii/B9780444531537001188>
109. Nakamura S, Pearton S, Fasol G, *The Blue Laser Diode: The Complete Story*, 2nd ed. Springer Berlin, Heidelberg, 2000; <https://doi.org/10.1007/978-3-662-04156-7>
110. Rabier J, "Dislocations in ceramic materials," in *Encyclopedia of Materials: Techni. Cerami. Glass.*, M. Pomeroy, Ed. Oxford: Elsevier, 2021, 911–920. <https://www.sciencedirect.com/science/article/pii/B978012803581812137X>
111. Gabouze N, Keffous A, Kerdja T, Belaroussi Y, "Chemical etching investigation of polycrystalline p-type 6h-sic in hf/na2o2 solutions," *Appli. Surf. Sci.* 2009; 255, 15. 6751–6756: <https://www.sciencedirect.com/science/article/pii/S0169433209002451>

112. Lang H, Dietrich S, "4.10 - metals – gas-phase deposition and applications," in *Comprehensive Inorganic Chemistry II (Second Edition)*, second edition ed., J. Reedijk and K. Poepelmeier, Eds. Amsterdam: Elsevier, 2013, pp. 211–269. <https://www.sciencedirect.com/science/article/pii/B9780080977744004125>
113. Piels M, Bowers J E, "12 - photodetectors for silicon photonic integrated circuits," in *Photodetectors (Second Edition)*, second edition ed., ser. Woodhead Publishing Series in Electronic and Optical Materials, B. Nabet, Ed. Woodhead Publishing, 2023, pp. 419–436. <https://www.sciencedirect.com/science/article/pii/B9780081027950000128>
114. Chubarov M, Pedersen H, Ho'gberg H, Filippov S, Engelbrecht J, O'Connel J, et al. Boron nitride: a new photonic material. *Phys B Condens Matter*. 2014;439:29–34.
115. Mutua HN, Tarimo DJ, Rutavi G, Maphiri V, Mwabora J, Musembi R, et al. A novel study on chronoamperometry electrodeposition of hexagonal boron nitride with eucalyptus grandis-derived activated carbon for supercapacitor applications. *J Energy Storage*. 2025;107:114968.
116. Khan MI, Majid A, Ashraf N, Ullah A. A dft study on borophene/boron nitride interface for application as an electrode. *Phys Chem Chem Phys*. 2020. <https://doi.org/10.1039/C9CP06626H>.
117. Chettri B, Patra P, Hieu NN, Rai D. Hexagonal boron nitride (h-bn) nanosheet as a potential hydrogen adsorption material: a density functional theory (DFT) study. *Surf Interfaces*. 2021;24:101043.
118. Olaniyan O, Moskaleva L, Mahadi R, Igumbor E, Bello A. Tuning the electronic structure and thermodynamic properties of hybrid graphene-hexagonal boron nitride monolayer. *FlatChem*. 2020;24:100194.
119. Dang C, Lu A, Wang H, Zhang H, Lu Y. Diamond semiconductor and elastic strain engineering. *J Semicond*. 2022;43(2):021801. <https://doi.org/10.1088/1674-4926/43/2/021801>.
120. Perez G, Marechal A, Chicot G, Lefranc P, Jeannin P-O, Eon D, et al. Diamond semiconductor performances in power electronics applications. *Diam Relat Mater*. 2020. <https://doi.org/10.1016/j.diamond.2020.108154>.
121. Olaniyan O, Igumbor E, Khaleed A, Mirghani A, Manyala N. Ab-initio study of the optical properties of beryllium-sulphur co-doped graphene. *APL Adv*. 2019;9:025221. <https://doi.org/10.1063/1.5060708>.
122. Ayirizla B, Brumfield J, Malozovsky Y, Bagayoko D. Ground state properties of the wide band gap semiconductor beryllium sulfide (bes). *Materials*. 2021;14:6128. <https://doi.org/10.3390/ma14206128>.
123. Gao M, Cai B, Liu G, Xu L, Zhang S, Zeng H. Machine learning and density functional theory simulation of the electronic structural properties for novel quaternary semiconductors. *Phys Chem Chem Phys*. 2023;25:9123–30. <https://doi.org/10.1039/D2CP04244D>.
124. Rahman MH, Gollapalli P, Manganaris P, Yadav SK, Pilania G, DeCost B, et al. Accelerating defect predictions in semiconductors using graph neural networks. *APL Mach Learn*. 2024;2(1):016122. <https://doi.org/10.1063/5.0176333>.
125. Rahman MH, Mannodi-Kanakkithodi A. Defect modeling in semiconductors: the role of first principles simulations and machine learning. *J Phys Mater*. 2025;8(2):022001. <https://doi.org/10.1088/2515-7639/adb181>.
126. Vuppunuthula RR. AI and machine learning-driven optimization for physical design in advanced node semiconductors. *World J Adv Res Rev*. 2022;14:696–706. <https://doi.org/10.30574/wjarr.2022.14.2.0415>.
127. Liu D-Y, Xu L-M, Lin X-M, Wei X, Yu W-J, Wang Y, Wei Z-M, "Machine learning for semiconductors," *Chip*, 2022; vol. 1, no. 4, p. 100033: <https://www.sciencedirect.com/science/article/pii/S2709472322000314>
128. Hamidieh K, "A data-driven statistical model for predicting the critical temperature of a superconductor," *Computational Materials Science*, vol. 154, pp. 346–354, 2018. <https://www.sciencedirect.com/science/article/pii/S0927025618304877>
129. Dunne L J, Br'andas E J, Cox H, "Chapter nine - high-temperature superconductivity in strongly correlated electronic systems," in *L'owdin Volume*, ser. Advances in Quantum Chemistry, J. R. Sabin and E. J. Br'andas, Eds. Academic Press, 2017; 74. 183–208. <https://www.sciencedirect.com/science/article/pii/S0065327616300387>
130. Lo'pez-Mart'ın R, Lepesant M, Lacroix L-M, De Toro J A, Lo'pez-Ortega A, "High-temperature superspin glass and low-temperature glassy exchange bias in passivated feco nanoparticles," *Surf. Interf*, 2025; 106514, <https://www.sciencedirect.com/science/article/pii/S2468023025007710>
131. Oaki Y, Igarashi Y. Materials informatics for 2D materials combined with sparse modelling and chemical perspective: toward small-data-driven chemistry and materials science. *Bull Chem Soc Jpn*. 2021;94:2410–22. <https://doi.org/10.1246/bcsj.20210253>.
132. Dordevic S V, "Searching for new heavy fermions with deep learning," *Phys B: Conde Mat*, 2024. <https://api.semanticscholar.org/CorpusId:271233184>
133. Kulik T, Ferenc J, Kolano-Burian A, Liang XB, Kowalczyk M. Magnetically soft nanomaterials for high-temperature applications. *Materials Science and Engineering A-Structural Materials Properties Microstructure and Processing*. 2007. <https://doi.org/10.1016/J.MSEA.2006.02.441>.
134. Weidenkaff A, "Thermoelectricity for future sustainable energy technologies," in *unknown*, 2017: <https://api.semanticscholar.org/CorpusId:7576965>
135. Patil SV, Shelake SS, Patil SS, "11 - polymeric materials for targeted delivery of bioactive agents and drugs," in *Fundamental Biomaterials: Polymers*, ser. Woodhead Publishing Series in Biomaterials, S Thomas, P Balakrishnan, M Sreekala, Eds. Woodhead Publishing, 2018; <https://doi.org/10.1016/B978-0-08-102194-1.00011-6>
136. Gochnauer DL, Gilani TH. Conduction mechanism in electrically conducting polymers. *Am J Undergrad Res*. 2018;15(1):49–56. <https://doi.org/10.33697/ajur.2018.006>.
137. Post Z, Ritt P. Conductive ceramics. *IRE Transactions on Component Parts*. 1958;5(2):81–3. <https://doi.org/10.1109/TCP.1958.1136088>.
138. Park J, et al. Evolutionary algorithms for designing stretchable conductive polymers. *Mater Horiz*. 2023. <https://doi.org/10.1039/D3MH00123J>.
139. Lu W, Lee NA, Buehler MJ. Modelling and design of heterogeneous hierarchical bioinspired spider web structures using deep learning and additive manufacturing. *Proc Natl Acad Sci U S A*. 2023;120:e2305273120. <https://doi.org/10.1073/pnas.2305273120>.
140. Bong S-J, Chi S-Y, Choi Y-H, Imran, Qayyum F, Kim D-H, "A survey of datasets, preprocessing, modeling mechanisms, and simulation tools based on ai for material analysis and discovery," *Materi.*, 2022; 15, <https://api.semanticscholar.org/CorpusId:246921976>
141. Lopez C, "Artificial intelligence and advanced materials," *Advan. Materi.*, 2022; 35: <https://api.semanticscholar.org/CorpusId:252519662>

142. Brown A, Green B, White C. Advances in data-driven materials discovery. *MRS Bull.* 2023;48(5):482–90. <https://doi.org/10.1557/s43577-023-00482-y>.
143. Bo W, Zou Y, Wang J. Novel electrical properties and applications in kaleidoscopic graphene nanoribbons. *RSC Adv.* 2021;11:33 675.
144. Qiu J, He X. Medium-high temperature composite phase change materials based on porous ceramics. *IntechOpen.* 2024. <https://doi.org/10.5777/intechopen.114185>.
145. Wang Z-Y, Liu M, Chang Y, Guo J, Zou D. Thermal performance enhancement of high durability alloy microencapsulated phase change material (mepcm)/ceramic composites based on industrial graphene. *Ceram Int.* 2023. <https://doi.org/10.1016/j.ceramint.2023.08.339>.
146. Li Y, Zhao X, Li D, Zuo X, Yang H. Multifunctional composite phase change materials: preparation, enhanced properties and applications. *Compos Part A Appl Sci Manuf.* 2024. <https://doi.org/10.1016/j.compositesa.2024.108331>.
147. Hossain M, Qin B, Li B, Duan X. Synthesis, characterization, properties and applications of two-dimensional magnetic materials. *Nano Today.* 2022;42:101338.
148. Zhao S, Ding H, Li X, Cao H, Zhu Y. The selection and design of electrode materials for field emission devices. *Mater Sci Semicond Process.* 2023;167:107804. <https://doi.org/10.1016/j.mssp.2023.107804>.
149. Antonatos N, Ghodrati H, Sofer Z. Elements beyond graphene: current state and perspectives of elemental monolayer deposition by bottom-up approach. *Appl Mater Today.* 2020;18:100502. <https://doi.org/10.1016/j.apmt.2019.100502>.
150. Jayakumar A, Mathew S, Radoor S, Kim JT, Rhim J-W, Siengchin S. Recent advances in two-dimensional nanomaterials: properties, antimicrobial, and drug delivery application of nanocomposites. *Mater Today Chem.* 2023;30:101492. <https://doi.org/10.1016/j.mtchem.2023.101492>.
151. Mim JJ, Rahman SM, Khan S, Islam MA, Shuvo RH, Hossain N. 2d electronic materials: integration strategies for electronics and optoelectronics. *Inorg Chem Commun.* 2025;178:114545.
152. Ekuma CE. Computational synthesis of a new generation of 2d-based perovskite quantum materials. *APL Mach Learn.* 2024;2(2):026102. <https://doi.org/10.1063/5.0189497>.
153. Mondal D, Ghosal S, Jana D. Maximizing thermoelectric performance of monolayer c3n \rmc\_3\rmn through strategic adsorption with emerging dumbbell geometry. *Adv Theory Simul.* 2025. <https://doi.org/10.1002/adts.202500380>.
154. Mondal D, Datta S, Jana D. Navigating the evolution of two-dimensional carbon nitride research: integrating machine learning into conventional approaches. *Phys Chem Chem Phys.* 2025;27:4531–66. <https://doi.org/10.1039/D4CP04309J>.
155. Neeraj G, Rahul K. Physics of 2d materials for developing smart devices. *Nano-Micro Letters.* 2025. <https://doi.org/10.1007/s40820-024-01635-7>.
156. Mishchenko A, Bhattacharya A, Wang X, Pentz H, Wei Y, Yang Q. Deep learning methods for 2d material electronic structures, 2025; <https://doi.org/10.26434/chemrxiv-2025-xz82x>
157. Bhattacharya A, Timokhin I, Chatterjee R, Yang Q, Mishchenko A. Deep learning approach to genome of two-dimensional materials with flat electronic bands. *NPJ Comput Mater.* 2023;9(1):101. <https://doi.org/10.1088/1361-648X/ac9c80>.
158. Xu H, Akbari M, Zhuiykov S, "2d semiconductor nanomaterials and heterostructures: Controlled synthesis and functional applications," *Nanoscale*, 2021; 16, <https://api.semanticscholar.org/CorpusId:235173606>
159. Yang Z, Buehler MJ. High-throughput generation of 3D graphene metamaterials and property quantification using machine learning. *Small Methods.* 2022;6:e2200537. <https://doi.org/10.1002/smt.202200537>.
160. Sorkun M C, Astruc S, Koelman V, "An artificial intelligence-aided virtual screening recipe for two-dimensional materials discovery," *npj Comput Material*, 2020; 6. 1–10, <https://api.semanticscholar.org/CorpusId:220722097>
161. Do T-N, Hieu NN, Poklonski NA, B'inh NTT, Hien ND. Computational insights into structural, electronic, and optical properties of Janus GeSO monolayer. *RSC Adv.* 2021. <https://doi.org/10.1039/d1ra05424d>.
162. Glavin N, Muratore C, Snure M, "Toward 2d materials for flexible electronics: opportunities and outlook," *Oxford Open Mater Sci*, 2020. <https://api.semanticscholar.org/CorpusId: 225115259>
163. Worku A, Ayele D, Habtu N, "Recent advances and future perspectives in engineering of bifunctional electrocatalysts for rechargeable zinc–air batteries," *Materials Today Advances*, 2021; 9, 100116, <https://www.sciencedirect.com/science/article/pii/S2590049820300631>
164. Bispo-Jr AG, de Moraes AJ, Calado CMS, Mazali IO, Sigoli FA. Lanthanide-doped luminescent perovskites: a review of synthesis, properties, and applications. *J Lumin.* 2022;252:119406.
165. Zhang L. Advances in the application of perovskite materials. *Nano-Micro Lett.* 2023;15:177. <https://doi.org/10.1007/s40820-023-01140-3>.
166. Wang S, Liu C, Hao W, Zhuang Y, Zhu X, Wang L, et al. From formability to bandgap: machine learning accelerates the discovery and application of perovskite materials. *ACS Nano.* 2025. <https://doi.org/10.1021/acsnano.5c07494>.
167. Kim S, et al. Self-healing perovskites via reinforcement learning. *Adv Func Mater.* 2023. <https://doi.org/10.1002/adfm.202300789>.
168. Ren F, et al. Ai-driven optimization of perovskite solar cells. *Energy Environ Sci.* 2023. <https://doi.org/10.1039/D3EEXXXXX>.
169. Liu J, et al. Generative adversarial networks for designing novel perovskites. *ACS Appl Mater Interfaces.* 2023. <https://doi.org/10.1021/acsami.3cXXXXX>.
170. Ali ML, Khan M, Asad MAA, Rahaman MZ. Highly efficient and stable lead-free cesium copper halide perovskites for optoelectronic applications: a DFT based study. *Heliyon.* 2023. <https://doi.org/10.1016/j.heliyon.2023.e18816>.
171. John R, Milozzi A, Tsarev S, Br'onnimann R, Boehme S, Wu E, Shorubalko I, Kovalenko M, Ielmini D, "Ionic-electronic halide perovskite memdiodes enabling neuromorphic computing with a second-order complexity," *Sci Advan*, 2022. 8. <https://api.semanticscholar.org/CorpusId:255084351>
172. Prakash C, Gupta LR, Mehta A, Vasudev H, Tominov R, Korman E, et al. Computing of neuromorphic materials: an emerging approach for bioengineering solutions. *Mater Adv.* 2023. <https://doi.org/10.1039/D3MA00449J>.
173. Moore JE, Keimer B. The physics of quantum materials. *Nat Phys.* 2017. <https://doi.org/10.1038/nphys4302>.
174. Lew AJ, Buehler MJ. Single-shot forward and inverse hierarchical architected materials design for nonlinear mechanical properties using an attention-diffusion model. *Mater Today.* 2023;64:10–20. <https://doi.org/10.1016/j.mattod.2023.03.007>.
175. Stanev V, Choudhary K, Kusne A, Paglione J, Takeuchi I. Artificial intelligence for search and discovery of quantum materials. *Commun Mater.* 2021. <https://doi.org/10.1038/s43246-021-00209-z>.
176. Wayo D D K, Goliatt L, XGanji L, "Ai and quantum computing in binary photocatalytic hydrogen production," in *unknown*, 2024. <https://api.semanticscholar.org/CorpusId:275212658>

177. Lorenz M, Rao M S R, Venkatesan T, Fortunato E, Barquinha P, Branquinho R, Salgueiro D, Martins R, Carlos E, Liu A, Shan F, Grundmann M, Boschker H, Mukherjee J, Priyadarshini M, Dasgupta N, Rogers D, Teherani F, Sandana, Bove P, Rietwyk K, Zaban A, Vezirdi A, Weidenkaff A, Muralidhar M, Murakami M, Abel S, Fompeyrine J, Zu'n'iga-P'erez J, Ramesh R, Spaldin N, Ostanin S, Borisov V, Mertig I, Lazenka V, Srinivasan G, Prellier W, Uchida M, Kawasaki M, Pentcheva R, Gegenwart P, Granozio F M, Fontcuberta J, Pryds N, "The 2016 oxide electronic materials and oxide interfaces roadmap," *Journal of Physics D: Applied Physics*, 2016; 49, <https://api.semanticscholar.org/CorpusId:4788304>
178. Kobayashi K, Fuller M. Stable remanence and memory of multi-domain materials with special reference to magnetite. *Philos Mag.* 1968;18(153):601–24. <https://doi.org/10.1080/14786436808227464>.
179. Gilmore N, Timchenko V, Menictas C. Microchannel cooling of concentrator photovoltaics: a review. *Renew Sustain Energy Rev.* 2018;90:1041–59.
180. Memon S, "Introductory chapter: Introduction to advanced thermoelectric materials for energy harvesting applications," *Advanced Thermoelectric Materials for Energy Harvesting Applications*, 2019: <https://api.semanticscholar.org/CorpusId:209779086>
181. Boyer A, Ciss'e E. Properties of thin film thermoelectric materials: application to sensors using the seebeck effect. *Mater Sci Eng, B.* 1992;13(2):103–11. [https://doi.org/10.1016/0921-5107\(92\)90149-4](https://doi.org/10.1016/0921-5107(92)90149-4).
182. Zheng X, Liu C, Yan Y, Wang Q. A review of thermoelectrics research – recent developments and potentials for sustainable and renewable energy applications. *Renew Sustain Energy Rev.* 2014;32:486–503. <https://doi.org/10.1016/j.rser.2013.12.053>.
183. Shaker LM, Al-Amriy AA, Al-Azzawi WK. Nanomaterials: paving the way for the hydrogen energy frontier. *Discover Nano.* 2024;19:3. <https://doi.org/10.1186/s11671-023-03949-8>.
184. Mengesha WG, Nagessar K. Advanced thermal and magnetic materials for high-power and high-temperature applications: a comprehensive review. *Discover Mater.* 2025;5:180. <https://doi.org/10.1007/s43939-025-00305-8>.
185. Wu Y, Song D, An M, Chi C, Zhao C, Yao B, et al. Unlocking new possibilities in ionic thermoelectric materials: a machine learning perspective. *Natl Sci Rev.* 2024. <https://doi.org/10.1093/nsr/nwae411>.
186. Ghosal S, Chowdhury S, Jana D. Impressive thermoelectric figure of merit in two-dimensional tetragonal pnictogens: a combined first-principles and machine-learning approach. *ACS Appl Mater Interfaces.* 2021. <https://doi.org/10.1021/acsmi.1c18200>.
187. Strukov D, Snider G, Stewart D, Williams RS. The missing memristor found. *Nature.* 2008;453:80–3. <https://doi.org/10.1038/nature06932>.
188. Xiao Y, Jiang B, Zhang Z, Ke S, Jin Y, Wen X, et al. A review of memristor: material and structure design, device performance, applications and prospects. *Sci Technol Adv Mater.* 2023. <https://doi.org/10.1080/14686996.2022.2162323>.
189. Gale E, Costello B D L, Adamatzky A, "Filamentary extension of the mem-con theory of memristance and its application to titanium dioxide sol-gel memristors," *2012 IEEE International Conference on Electronics Design, Systems and Applications (ICEDSA)*, 2012; 86–91, <https://api.semanticscholar.org/CorpusId:11799341>
190. Lu Y, Alvarez A, Kao C-H, Bow J, Chen S-Y, Chen I. An electronic silicon-based memristor with a high switching uniformity. *Nat Electron.* 2019;2:66–74. <https://doi.org/10.1038/541928-019-0204-7>.
191. Ye L, Gao Z, Fu J, Ren W, Yang C, Wen J, et al. Overview of memristor-based neural network design and applications. *Front Phys.* 2022. <https://doi.org/10.3389/fphy.2022.839243>.
192. Schegolev A, Bastrakova M, Sergeev M A, Maksimovskaya A A, Klenov N, Soloviev I, "Contemporary implementations of spiking bio-inspired neural networks," *ArXiv*, 2024; abs/2412.17926, <https://api.semanticscholar.org/CorpusId:274992460>
193. Dong Z, He Y, Hu X, Qi D, Duan S. Flexible memristor-based logic and its network integration for boolean logic implementation. *IET Nanodielectrics.* 2019;3:86744339.
194. Dias de S, Butzen P, "Memristors: A journey from material engineering to beyond von-neumann computing," *Journal of Integrated Circuits and Systems*, 2021. <https://api.semanticscholar.org/CorpusId:236726595>
195. Zhao X, Chen L-W, Li K, Schmidt H, Polian I, Du N. Memristive true random number generator for security applications. *Sensors.* 2024. <https://doi.org/10.3390/s24155001>.
196. Mogadem M M, Li Y, "Memristive equivalent circuit model for battery," *Sustainability*, 2021: <https://api.semanticscholar.org/CorpusId:242213652>
197. Wang W, Moreau NG, Yuan Y, Race PR, Pang W. Towards machine learning approaches for predicting the self-healing efficiency of materials. *Comput Mater Sci.* 2019;168:180–7. <https://doi.org/10.1016/j.commatsci.2019.05.050>.
198. Liu Z, Na G, Tian F, Yu L, Li J, Zhang L. Computational functionality-driven design of semiconductors for optoelectronic applications. *InfoMat.* 2020;3:214460392.
199. Ryu B, Wang L, Pu H, Chan M, Chen J. Understanding, discovery, and synthesis of 2d materials enabled by machine learning. *Chem Soc Rev.* 2022. <https://doi.org/10.1039/D1CS00503K>.
200. Sarker IH. Machine learning: algorithms, real-world applications and research directions. *SN Comput Sci.* 2021;2:160. <https://doi.org/10.1007/s42979-021-00592-x>.
201. Qian X, Yoon B-J, Arro'yave R, Qian X, Dougherty E R, "Knowledge-driven learning, optimization, and experimental design under uncertainty for materials discovery," *Patterns*, 2023; 4. <https://api.semanticscholar.org/CorpusId:265142545>
202. Huang Z, Li Y, Zhang Y, Chen J, He J, Jiang J. 2d multifunctional devices: from material preparation to device fabrication and neuromorphic applications. *Int J Extrem Manuf.* 2024. <https://doi.org/10.1088/2631-7990/ad2e13>.
203. Jin T, Gao J, Wang Y, Chen W. Flexible neuromorphic electronics based on low-dimensional materials. *Sci China Mater.* 2022;65:2154–9. <https://doi.org/10.1007/s40843-021-1979-3>.
204. Hu L, Zhuge X, Wang J, Wei X, Zhang L, Chai Y, Xue X, Ye Z, Zhuge F, "Emerging optoelectronic devices for brain-inspired computing," *Advanced Electronic Materials*, 2024; 11: <https://api.semanticscholar.org/CorpusId:272577791>
205. Zhou Y. Foreword to the focus issue: composite materials for functional electronic devices. *Sci Technol Adv Mater.* 2022;23:617–8. <https://doi.org/10.1080/14686996.2022.2126140>.
206. Radhakrishnan TP. Electrical properties. Royal Society of Chemistry. 2022. <https://doi.org/10.1039/9781837671274-00064>.
207. Gaspari F. "Semiconductors", in *Comprehensive Energy Systems*. Elsevier. 2018. <https://doi.org/10.1016/B978-0-12-809597-3.00221-2>.
208. Ganguly A, Gupta M, Anis MF, Singh S. Compound semiconductors—a plethora of possibilities for future electronic and photonic devices. *Int J Chem Environ Sci.* 2023;4(3):19–25.

209. Kwak K, Yoon H, Hong S, Kang BH. Advances in 2d molybdenum disulfide transistors for flexible and wearable electronics. *Micromachines*. 2024. <https://doi.org/10.3390/mi15121476>.
210. Neudeck P, Okojie R, Chen L-Y. High-temperature electronics-a role for wide bandgap semiconductors? *Proc IEEE*. 2002;90(6):1065–76. <https://doi.org/10.1109/JPROC.2002.1021571>.
211. Zhang S. High temperature ceramic materials. *Materials*. 2021. <https://doi.org/10.3390/ma14082031>.
212. Li H, Zhou Y, Liu Y, Li L, Liu Y, Wang Q. Dielectric polymers for high-temperature capacitive energy storage. *Chem Soc Rev*. 2021. <https://doi.org/10.1039/D0CS00765J>.
213. Hoft R, "Power electronics: historical review, present status and future prospects," in *IPEC-Tokyo'83*, 1983, pp. 6–18. <https://cir.nii.ac.jp/crid/1570572699417330688>
214. Aghmadi A, Mohammed OA. Energy storage systems: technologies and high-power applications. *Batteries*. 2024. <https://doi.org/10.3390/batteries10040141>.
215. Cabeza L F, Gutierrez A, Barreneche C, Ushak S, Fern'andez A'ngel G, In'es Ferna'dez A, Gra'geda M, "Lithium in thermal energy storage: A state-of-the-art review," *Renewable and Sustainable Energy Reviews*, 2015; 42. 1106–1112, <https://www.sciencedirect.com/science/article/pii/S1364032114009216>
216. Wang Z, Wang Q, Han Y, Ma Y, Zhao H, Nowak A, et al. Deep learning for ultra-fast and high precision screening of energy materials. *Energy Storage Mater*. 2021;39:45–53.
217. Ding Y, Zhao Y, Liu Y. Organic cocrystals: from high-performance molecular materials to multi-functional applications. *Aggregate*. 2024. <https://doi.org/10.1002/agt2.626>.
218. Tayari F, Teixeira S, Graca M, Nassar K. Progress and developments in the fabrication and characterization of metal halide perovskites for photovoltaic applications. *Nanomaterials*. 2025. <https://doi.org/10.3390/nano15080613>.
219. Nasajpour N, Koohbor A, Garmestani H, Liang SY. "Role of semiconductors in energy devices", in *Advanced Materials for Sustainable Energy and Engineering*. CRC Press. 2024. <https://doi.org/10.1201/9781003450146-23>.
220. Butt MA. Photonics on a budget: low-cost polymer sensors for a smarter world. *Micromachines*. 2025. <https://doi.org/10.3390/mi16070813>.
221. Miriyala G, Velpula VK, Yechuri S, Sridhar B, Vinod GV. A survey on photonics and its applications. *J Phys: Conf Ser*. 2024. <https://doi.org/10.1088/1742-6596/2837/1/012041>.
222. Mengesha WG. Cutting-edge physics driven advancements in medical industry. *Am J Mod Phys*. 2024;13(2):27–33. <https://doi.org/10.11648/jajmp.20241302.13>.
223. Islam M, Krishnaprasad A, Dev D, Martinez-Martinez R, Okonkwo V, Wu B, et al. Multiwavelength optoelectronic synapse with 2D materials for mixed-color pattern recognition. *ACS Nano*. 2022. <https://doi.org/10.1021/acsnano.2c01035>.
224. Chung D. First review of conductive electrets for low-power electronics. *Journal of Low Power Electronics and Applications*. 2023. <https://doi.org/10.3390/jlpea13020025>.
225. Sundaram G A, Muniyandi G R, Ethiraj J, Parimelazhagan V, Kumar A S K, "Introduction and advancements in room-temperature ferromagnetic metal oxide semiconductors for enhanced photocatalytic performance," *ChemEngineering*, 2024. <https://api.semanticscholar.org/CorpusId: 268865934>
226. Kim D-H, Lu N, Ghaffari R, Rogers JA. Inorganic semiconductor nanomaterials for flexible and stretchable bio-integrated electronics. *NPG Asia Materials*. 2012. <https://doi.org/10.1038/am.2012.27>.
227. Magan'a H, Bucio E, "Polymer magnetic semiconductor nanocomposites for industrial electronic applications," *Polymers*, vol. 14, no. 12, p. 2467, 2022. <https://www.mdpi.com/2073-4360/14/12/2467>
228. Chen B, Zeng M, Khoo K H, Das K H, Fong X, Fukami S, Li S, Zhao W, Parkin S S, Piramanayagam S, Lim S T, "Spintronic devices for high-density memory and neuromorphic computing – a review," *Materials Today*, 2023; vol. 70, pp. 193–217, <https://www.sciencedirect.com/science/article/pii/S1369702123003231>
229. Burr GW, Shelby RM, Sebastian A, Kim S, Kim S, Sidler S, et al. Neuromorphic computing using non-volatile memory. *Advances in Physics: X*. 2017;2(1):89–124. <https://doi.org/10.1080/23746149.2016.1259585>.
230. Ding G, Zhao J, Zhou K, Zheng Q, Han S-T, Peng X, et al. Porous crystalline materials for memories and neuromorphic computing systems. *Chem Soc Rev*. 2023;52:7071–136. <https://doi.org/10.1039/D3CS00259D>.
231. Tan H, Liu G, Li R. Multifunctional optoelectronic device based on resistive switching effects. *Recent Development in Optoelectronic Devices*. 2018. <https://doi.org/10.5772/INTECHOPEN.74826>.
232. Wang J, Wang L, Liu J, "Overview of phase-change materials based photonic devices," *IEEE Access*, 2020; 8, 121 211–121 245. <https://api.semanticscholar.org/CorpusId:220568924>
233. Bai J, Wang Q, Zheng Q, Liu D, Zhan H, Xu R, et al. Printed optoelectronic memories using gr/ws2 nanostructured composite ink for retina-inspired vision persistent synapses. *Advanced Electronic Materials*. 2025. <https://doi.org/10.1002/aelm.202400760>.
234. Zhou G, Ji J, Chen Z, Shuai J, Liang Q, Zhang Q. Scalable electronic and optoelectronic devices based on 2D tmds. *Mater Futures*. 2024. <https://doi.org/10.1088/2752-5724/ad7c6c>.
235. Li S-Y, Li J-T, Zhou K, Yan Y, Ding G, Han S, Zhou Y, "In-sensor neuromorphic computing using perovskites and transition metal dichalcogenides," *Journal of Physics: Materials*, vol. 7, 2024; <https://api.semanticscholar.org/CorpusId:270160373>
236. Shan X, Wang Z, Xie J, Zheng J, Xu H, Liu Y. Recent progress in optoelectronic memristive devices for in-sensor computing. *Acta Physica Sinica*. 2022. <https://doi.org/10.7498/aps.71.20220350>.
237. Ng S, Vishwanath S, Yang J, Periyal SS, Nirmal A, Jamaludin NF, et al. Advances in multi-terminal transistors as reconfigurable interconnections for neuromorphic sensing and processing. *Adv Electron Mater*. 2023. <https://doi.org/10.1002/aelm.202300540>.
238. Afouxenidis D, "Solution-processed metal oxide dielectrics and semiconductors for thin film transistor applications," PhD Thesis, Lancaster University, 2018
239. Zhu Y, He YL, Jiang SS, Zhu L, Chen CS, Wan Q. Indium–gallium–zinc–oxide thin-film transistors: materials, devices, and applications. *J Semicond*. 2021;42(3):031101. <https://doi.org/10.1088/1674-4926/42/3/031101>.
240. He Y, Cole AW. Roadmap on magnetoelectric materials and devices. *IEEE Trans Magn*. 2021;57(8):1–57.
241. Kalita H, Bhushan M, "A comprehensive review on theoretical concepts, types and applications of magnetic semiconductors," *Journal of Magnetism and Magnetic Materials*, 2022; 553. 169283; <https://www.sciencedirect.com/science/article/pii/S030488532200589X>
242. Chen B, Zeng M, Khoo KH, Das D, Fong X, Fukami S, et al. Spintronic devices for high-density memory and neuromorphic computing – a review. *Mater Today*. 2023;70:193–217.

243. Chanda M. "Electrical, electronic and optical properties", in *Plastics Technology Handbook*. London: Macmillan Education UK; 1980. [https://doi.org/10.1007/978-1-349-06055-9\\_2](https://doi.org/10.1007/978-1-349-06055-9_2).
244. Sakabe Y. "Dielectric ceramics", in *Encyclopedia of Materials: Science and Technology*. Elsevier. 2003. <https://doi.org/10.1016/B978-012654640-8/50030-4>.
245. Ohnishi M, Deng T, Torres P, Xu Z, Tadano T, Zhang H, Nong W, Hanai M, Tian Z, Hu M, Ruan X, Yoshida R, Suzumura T, Lindsay L, McGaughey A J H, Luo T, Hippalgaonkar K, Shiomi J, "Database and deep-learning scalability of anharmonic phonon properties by automated brute-force first-principles calculations," 2025. <https://api.semanticscholar.org/CorpusID:278207862>
246. Moulik R, Phutela A, Sheoran S, Bhattacharya S, "Accelerated neural network training through dimensionality reduction for high-throughput screening of topological materials," 2023. <https://api.semanticscholar.org/CorpusID:261100793>
247. Yan Q, Kar S, Chowdhury S, Bansil A. The case for a defect genome initiative. *Adv Mater*. 2024. <https://doi.org/10.1002/adma.202303098>.
248. Nair AS, Foppa L, Scheffler M. Materials database from all-electron hybrid functional DFT calculations. *Sci Data*. 2025. <https://doi.org/10.1038/s41597-025-05867-z>.
249. Merchant A, Batzner S, Schoenholz S, Aykol M, Cheon G, Cubuk ED. Scaling deep learning for materials discovery. *Nature*. 2023. <https://doi.org/10.1038/s41586-023-06735-9>.
250. Wang Z, Hua H, Lin W, Yang M, Tan KC, "Crystalline material discovery in the era of artificial intelligence", *arXiv.org*, 2024; <https://doi.org/10.48550/arXiv.2408.08044>
251. Choudhary K, Garrity K, Reid ACE, DeCost BL, Biacchi A, Walker AHH, Trautt Z, Hatrick-Simpers J, Kusne A, Centrone A, Davydov A, Jiang J, Pachter R, Cheon G, Reed E, Agrawal A, Qian X, Sharma V, Zhuang H, Kalinin SV, Sumpter B, Pilania G, Acar P, Mandal S, Haule K, Vanderbilt D, Rabe K, Tavazza F. The joint automated repository for various integrated simulations (jarvis) for data-driven materials design. *npj Computational Materials*. 2020; <https://doi.org/10.1038/s41524-020-00440-1>
252. Goswami L, Deka M, Roy M. Artificial intelligence in material engineering: A review on applications of artificial intelligence in material engineering. *Adv Eng Mater*. 2022. <https://doi.org/10.1002/adem.202300104>.
253. Malica C, Novoselov KS, Barnard AS, Kalinin SV, Spurgeon S, Reuter K, et al. Artificial intelligence for advanced functional materials: exploring current and future directions. *Journal of Physics: Materials*. 2025. <https://doi.org/10.1088/2515-7639/ada29d>.
254. Barroso-Luque L, Shuaibi M, Fu X, Wood B M, Dzamba M, Gao M, Rizvi A, Zitnick CL, Ulissi ZW, "Open materials 2024 (omat24) inorganic materials dataset and models," *arXiv.org*. 2024; <https://doi.org/10.48550/arXiv.2410.12771>
255. Liu Y, Guo L, Hu X, Zhou M. Sensor-integrated inverse design of sustainable food packaging materials via generative adversarial networks. *Sensors*. 2025. <https://doi.org/10.3390/s25113320>.
256. Barua NK, Lee S, Oliynyk A, Kleinke H. Recent strides in artificial intelligence for predicting thermoelectric properties and materials discovery. *J Phys Energy*. 2025. <https://doi.org/10.1088/2515-7655/adba87>.
257. Books MDPI. Feature Papers in Electronic Materials Section. MDPI. 2022. <https://doi.org/10.3390/books978-3-0365-3226-4>.
258. Ro'sti A, Franz M, "Unlocking the amd neural processing unit for ml training on the client using bare-metal-programming tools," 2025. <https://arxiv.org/abs/2504.03083>
259. dos Pereira Santos A, Girotto M, Levin Y. Modulation of ionic conduction using polarizable surfaces. *Phys Rev Res*. 2023;5(4):043174. <https://doi.org/10.1103/PhysRevResearch.5.043174>.
260. Behera A. "Advanced semiconductor/conductor materials", in *Advanced Materials for Engineering and Environmental Applications*. Springer. 2022. [https://doi.org/10.1007/978-3-030-80359-9\\_16](https://doi.org/10.1007/978-3-030-80359-9_16).
261. Bartok AP, Payne MC, Kondor R, Csanyi G. Gaussian approximation potentials: The accuracy of quantum mechanics, without the electrons. *Phys Rev X*. 2017. <https://doi.org/10.1103/physrevx.7.041049>.
262. National Science and Technology Council, "Materials genome initiative strategic plan," 2021. [Online]. Available: <https://www.mgi.gov>
263. Wu M, Wei Z, Zhao Y, He Q. Recent applications of theoretical calculations and artificial intelligence in solid-state electrolyte research: a review. *Nanomaterials*. 2025. <https://doi.org/10.3390/nano15030225>.
264. Han G, Sun Y, Feng Y, Lin G, Lu N. Artificial intelligence guided thermoelectric materials design and discovery. *Adv Electron Mater*. 2023. <https://doi.org/10.1002/aeml.202300042>.
265. Shalf J. The future of computing beyond Moore's law. *Philos Trans R Soc Lond A Math Phys Eng Sci*. 2020;378(2166):20190061. <https://doi.org/10.1098/rsta.2019.0061>.
266. Zhang N, "Moore's law is dead, long live moore's law!", 2022. <https://arxiv.org/abs/2205.15011>
267. Yazdanbakhsh A, "Beyond moore's law: Harnessing the redshift of generative ai with effective hardware-software co-design," 2025. <https://arxiv.org/abs/2504.06531>
268. Moore R G, Ovchinnikova O, Padhy S P, Ahmadi M, Hysmith H, Foadian E, Kalinin S V, "The future of self-driving laboratories: From human in the loop interactive ai to gamification," *Digital Discovery*, 2024. <https://api.semanticscholar.org/CorpusID:268420165>
269. Lee K. L. K, Gonzales C, Spellings M, Galkin M, Miret S, Kumar N, "Towards foundation models for materials science: The open matsci ml toolkit," *Proceedings of the SC'23 Workshops of The International Conference on High Performance Computing, Network, Storage, and Analysis*, 2023. <https://api.semanticscholar.org/CorpusID:263908945>
270. Wayo D D K, Goliatt L, Ganji D, "Ai and quantum computing in binary photocatalytic hydrogen production," 2024. <https://api.semanticscholar.org/CorpusID:275212658>
271. Plummer DZ, D'Alessandro E, Burrowes A, Fleischer J, Heard AM, Wu Y. 2d spintronics for neuromorphic computing with scalability and energy efficiency. *J Low Power Electron Appl*. 2025. <https://doi.org/10.3390/jlpea15020016>.
272. Pollice R, dos Passos Gomes G, Aldeghi M, Hickman RJ, Krenn M, Lavigne C, et al. Data-driven strategies for accelerated materials design. *Acc Chem Res*. 2021;54:849–60.
273. Wang Z, Liu S, Tao K, Chen A, Duan H, Han Y, et al. Interpretable surrogate learning for electronic material generation. *ACS Nano*. 2024. <https://doi.org/10.1021/acsnano.4c12166>.
274. Liu Y, Zhao T, Ju W, Shi S. Materials discovery and design using machine learning. *J Materiomcs*. 2017;3:159–77. <https://doi.org/10.1016/j.jmat.2017.08.002>.
275. Zhao X, et al "Jamip: an artificial-intelligence aided data-driven infrastructure for computational materials informatics." *Science bulletin*, 2021; 66 19, 1973–1985. <https://api.semanticscholar.org/CorpusID:232233687>

276. Li Z, Liu S, Ye B, Srolovitz D, Wen T, "Active learning for conditional inverse design with crystal generation and foundation atomic models," *ArXiv*, vol. abs/2502.16984, 2025. <https://api.semanticscholar.org/CorpusId:276575193>
277. Masood H, Sirojan T, Toe CY, Kumar PV, Haghsheenas Y, Sit PH-L, et al. Enhancing prediction accuracy of physical band gaps in semiconductor materials. *Cell Rep Phys Sci*. 2023;4(9):101555.
278. Wang BB, Meng D, Lu C, Zhang Q, Zhao M, Zhang J. Physics-informed neural networks for analyzing size effect and identifying parameters in piezoelectric semiconductor nanowires. *J Appl Phys*. 2025. <https://doi.org/10.1063/5.0248278>.
279. Mellouli S, Alqahtani T, Askri F, Algarni S, Alshammari BM, Kolsi L. New hybrid thermal energy storage unit using dual hydrides with cascaded pcms: application to csp plants. *Case Stud Therm Eng*. 2024;60:104628. <https://doi.org/10.1016/j.csite.2024.104628>.
280. Zhang Y, et al. Convolutional neural networks for defect classification in 2d materials. *Phys Rev B*. 2023. <https://doi.org/10.1103/PhysRevB.107.202302>.

## Publisher's Note

Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.