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Artificial Intelligence: Impact on the Development of Electrical Materials

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Abstract: *Electrical materials play a pivotal role in electrical engineering, yet conventional research methodologies relying on experimental approaches and theoretical calculations face challenges of low efficiency and high costs. The rapid advancement of artificial intelligence (AI) technology has introduced novel tools for electrical material research, significantly enhancing the efficiency of material design, performance prediction, and experimental optimization. This paper systematically reviews recent progress in AI applications across semiconductor, alloy, energy storage, and metallic materials. In semiconductor research, machine learning has improved analytical precision through optimization of Hubbard U parameters and prediction of perovskite defect transition levels. For alloy materials, AI combined with active learning strategies has accelerated the discovery and performance optimization of high-entropy alloys.Our analysis reveals that AI technology substantially reduces material development cycles and experimental costs through multi-source data integration, quantitative model construction, and multi-objective optimization strategies. Looking forward, with advancements in data science and computational capabilities, AI is poised to play an increasingly critical role in multi-scale material design, performance prediction, and novel material development for electrical engineering, thereby driving technological innovations in power and electronic systems.*

Keywords: *Artificial Intelligence，Electrical Materials，Machine Learning，Material Performance，Predictive Multi-Objective Optimization*

1.Introduction

Electrical engineering materials form the foundational elements of modern electrical systems, encompassing conductive materials, semiconductors, magnetic materials, and others, whose performance directly governs the efficiency of power generation, transmission, and utilization. Conventional research methodologies relying on experimental trial-and-error and theoretical modeling face significant challenges due to material complexity, resulting in prolonged development cycles and high costs. This necessitates the adoption of efficient and precise alternatives. Recent breakthroughs in artificial intelligence (AI) technologies have introduced paradigm-shifting advancements in materials science, particularly in data-driven material design, performance prediction, and experimental optimization.Nevertheless, critical challenges persist, including the curation of high-quality datasets, integration of multiscale models, and synergistic experimental validation. As computational power and

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algorithms evolve, AI is poised to exert profound impacts on the multidimensional design of electrical engineering materials, offering transformative solutions for energy, electronics, and quantum technologies.

2. Research status

2.1 Applications of Artificial Intelligence in Semiconductor Materials

Semiconductor materials, as the cornerstone of modern electronic devices, exhibit critical sensitivity where subtle variations in their properties can profoundly impact device performance. The integration of AI technologies in this field has not only enhanced the accuracy of material property predictions but also accelerated the discovery of novel materials. Through advanced machine learning algorithms, researchers can extract pivotal parameters from complex datasets, thereby optimizing material design and advancing semiconductor materials science.

Liu Hengyu[1]effectively addressed the self-interaction error in III-V semiconductor materials by implementing machine learning Bayesian optimization within the density functional theory framework incorporating Hubbard U correction (DFT+U). This approach provides a comprehensive methodology for enhanced precision. By optimizing Hubbard U parameters for 13 semiconductor materials through Bayesian machine learning and subsequent DFT+U implementation, the study rectified inherent errors in bandgap and electronic band structure descriptions arising from standard DFT calculations. Comparative analyses with HSE06 hybrid functional results and experimental data established a benchmark for optimal U parameter selection in III-V semiconductors. This methodology significantly mitigates computational limitations in III-V semiconductor research, injecting new momentum into previously constrained investigations.Wu Xiaoyu[2]pioneered a data-driven machine learning framework for predicting defect transition levels in perovskite materials. Through comparative analysis of three distinct machine learning models - K-nearest neighbors regression (KNR), support vector regression (SVR), and histogram gradient boosting regression (HGBR)-the study identified HGBR as the superior predictive model. Subsequent validation demonstrated its efficacy in predicting charge transition levels for two perovskite variants. This breakthrough provides novel insights for defect engineering in perovskite semiconductors, enhancing research efficiency and enabling customized material development. Such advancements hold substantial implications for optoelectronics, solar cell technology, and quantum computing applications.

Future research directions necessitate deeper integration of AI with quantum mechanical principles and statistical physics, particularly through multiscale modeling approaches to address interfacial heterostructures and non-equilibrium processes in semiconductors. Concurrently, developing interpretable machine learning models will be crucial for elucidating the physical mechanisms underlying material optimization, thereby facilitating a paradigm shift from empirical design to theory-guided material engineering. With continued algorithmic innovation and interdisciplinary collaboration, AI is poised to play pivotal roles in designing next-generation semiconductors (e.g., topological materials, two-dimensional materials), laying theoretical foundations for advanced electronic, photonic, and quantum devices.

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2.2 Applications of Artificial Intelligence in Alloy Materials

Performance optimization of alloy materials constitutes a complex process governed by multifaceted interactions. The integration of AI technologies has significantly enhanced the efficiency of this endeavor. Machine learning models empower researchers to identify critical governing factors from extensive experimental datasets, predict alloy properties, and thereby guide experimental design and material refinement, accelerating the discovery and application of novel alloy systems.

Seyedmehrab Hosseini[3] et al. employed machine learning to predict and optimize the hardness of Nb-Ti-V-Zr high-entropy refractory alloys. Their experimental investigations identified three critical descriptors-atomic size difference, configuration mixing entropy, and average electronegativity disparity -providing fundamental insights for hardness optimization in high-entropy refractory alloys. Ziyuan Rao et al. [4] developed an active learning strategy integrating machine learning with power function theory, thermodynamic calculations, and experimental validation to expedite high-entropy alloy discovery. Compared to conventional alloy design methodologies, their approach demonstrated superior efficiency in novel material identification while substantially reducing experimental costs and timelines. Similarly, Chonghang Zhao et al. [5] investigated metallic precursor dealloying through machine learning algorithms, predicting 132 potential ternary dealloying systems. Notably, only 59 systems satisfied conventional enthalpy-mixing criteria, highlighting the necessity of combining machine learning predictions with experimental verification to expand viable alloy systems.

Future advancements will require synergistic integration of AI with cross-scale simulation methodologies such as phase-field theory and molecular dynamics, enabling multiscale modeling frameworks bridging electronic structures to macroscopic properties. The development of interpretable machine learning architectures will elucidate the physical essence underlying descriptor-property correlations (e.g., dislocation dynamics, interface effects), driving a paradigm shift from "black-box prediction" to "mechanism-driven" alloy design. Furthermore, the implementation of generative models and reinforcement learning promises global optimization of composition-processing-property relationships, establishing novel pathways for theoretically designed ultrahigh-performance alloys. Through innovative algorithm development and deep convergence with multiphysics theories, AI will catalyze the transition from empirical exploration to rational design in alloy materials, delivering transformative material solutions for aerospace, energy infrastructure, and related strategic sectors.

2.3 Applications of Artificial Intelligence in Energy Storage Materials

The growing global energy demand has intensified the need for high -performance energy storage materials. The application of AI technologies, particularly through machine learning model development, provides innovative tools for advancing energy storage research. By leveraging big data analytics and machine learning frameworks, researchers can rapidly screen and design electrode/electrolyte materials with tailored properties, accelerating material discovery and technological innovation in energy storage systems.

Xu Jing and Wang Yuqi [6]et al. developed a multi-fidelity transfer framework integrated with machine learning models for secondary battery material simulations through big data methodologies. This approach enables rapid prediction of ion transport properties, enhancing understanding of material-battery performance correlations and facilitating the development of next-generation solid-state secondary battery materials. Bowen Deng[7] et al. introduced the Crystal Hamiltonian Graph

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Neural Network (CHGNet), a graph neural network-based machine-learned interatomic potential (MLIP) capable of simulating universal potential energy surfaces for large-scale systems with complex electronic interactions. CHGNet propagates atomic information via nodes and edges while preserving translational, rotational, and permutation invariances. It accepts crystal structures with unknown atomic charges as input and outputs corresponding energies, forces, stresses, and magnetic moments. By incorporating magnetic moments, CHGNet accurately captures electron orbital occupations, significantly enhancing its capacity to describe atomic and electronic degrees of freedom. Experimental validation demonstrated CHGNet's superior performance on the MPtrj dataset, exhibiting minimal mean absolute errors in energy, force, and stress predictions. Crucially, CHGNet successfully simulated ion rearrangements associated with charge transfer, providing critical insights into phase transitions in $LiMnO_2$ cathode materials. Chade Lv et al. [8] investigated machine learning (ML) applications in lithium-ion battery (LIB) material development and state prediction. ML implementations in LIBs primarily focus on two domains: predicting material properties and estimating battery states. ML models enable rapid screening of electrode/electrolyte materials with desired characteristics, while advanced battery management systems (BMS) utilize ML techniques for precise state-of-charge (SOC) and state-of-health (SOH) predictions. These advancements not only accelerate material discovery but also enhance LIB performance and safety through optimized battery management.

2.4 Applications of Artificial Intelligence in Metallic Materials

Metallic materials play pivotal roles in electrical and electronic systems. AI technologies, particularly machine learning algorithms, offer novel solutions for performance prediction and optimization of metallic materials. By analyzing vast experimental datasets, AI systems identify critical factors influencing material properties, enabling optimized designs that enhance performance and reliability.

Zhen-bing[9] et al. employed machine learning algorithms to predict electrical contact wear in brass materials, evaluating the effects of load, sliding velocity, displacement amplitude, current intensity, and surface roughness on contact resistance variations. They established predictive models using random forest (RF), support vector regression (SVR), and backpropagation neural network (BPNN) algorithms, trained and validated against experimental data. Their analysis revealed that increased load, current, and surface roughness reduce stabilized average resistance, whereas higher displacement amplitude and frequency elevate resistance. These findings provide a novel methodology for reliability assessment of electrical contact materials and wear-induced resistance prediction. Mi Zhishan[10] combined first-principles calculations with machine learning to investigate carbon content effects on hydrogen resistance in steel materials. They developed a high-accuracy machine learning force field (MLFF) for Fe-C-H systems using neural networks trained on ab initio molecular dynamics (AIMD) data, enabling precise predictions of atomic energies and forces. This framework offers a new tool for understanding hydrogen diffusion in steels and guides the design of hydrogen-resistant alloys. The methodology can be extended to explore other alloying elements' impacts, advancing theoretical foundations for high-strength low-alloy steel development. Yang Xufeng[11] proposed a Bayesian neural network (BNN) model for estimating P-S-N curves to predict metallic material fatigue life. By treating neural network weights as stochastic variables and employing Bayesian posterior distribution estimation, the BNN model not only predicts outcomes but also quantifies prediction uncertainties.

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This work expands machine learning applications in materials science while offering new perspectives for structural fatigue life analysis. Liu Shi and Huang Jiawei et al.[12] implemented deep potential (DP) models—a deep neural network-based interatomic potential—in ferroelectric material research. Their work demonstrated DP's efficacy in studying HfO_2-based ferroelectrics and classical perovskite systems, revealing microscopic mechanisms behind ultrahigh O^{2-} mobility in ferroelectric HfO_2 and flexoelectric/pyroelectric effects at $SrTiO_3$ polar domain boundaries. The DP framework significantly enhances simulation accuracy and efficiency, providing theoretical guidance for ferroelectric material design.

2.5 Applications of Artificial Intelligence in Emerging Materials

The application of AI technologies is expanding across diverse domains of electrical engineering materials, transcending limitations to specific material classes. By leveraging machine learning models and big data analytics, researchers can systematically analyze material properties from multifactorial perspectives, predict material behaviors, and deliver comprehensive guidance for material discovery, design, and application. These AI-driven approaches not only enhance research efficiency but also unlock novel possibilities for advancing electrical material science.

Delchere Don-tsa1[13]et al.employed supervised machine learning models integrated with density functional theory (DFT)-based high-throughput computations to predict Seebeck coefficients, electrical conductivities, and power factors of inorganic compounds. Their analysis revealed a strong correlation between thermoelectric performance and effective mass, leading to a machine learning model with 95% accuracy in identifying high-performance thermoelectric materials. This cluster-based predictive framework demonstrates exceptional robustness and precision in thermoelectric property evaluation, offering critical insights for optimizing thermoelectric material selection. Anna Stepashkina's team [14] investigated the influence of mechanical deformation (tensile strain) on electrical conductivity by developing a Boltzmann statistics-based predictive model, subsequently enhanced through coefficients derived from ensemble regression machine learning. Using composite films comprising polypropylene (PP) matrices, rubber, and carbon fillers (carbon black-CB, carbon nanofibers-CNF), they measured volume resistivity via four-probe methods to construct experimental datasets. The CatBoost regression algorithm was implemented to optimize Boltzmann-derived expressions for predicting resistance increases under operational stretching. Experimental validation demonstrated high-precision predictions of tensile-induced resistivity changes in thin-film materials. This methodology provides innovative strategies for forecasting conductivity degradation under mechanical stress.

3. Conclusions

AI technologies exhibit transformative potential in electrical material science, enabling accelerated material screening, precise property prediction, and substantial reductions in experimental costs and timelines. While conventional black-box models achieve high predictive accuracy, they often fail to elucidate the physical essence of material behaviors. Future advancements necessitate hybrid frameworks merging symbolic AI with deep learning—models that synergize data-driven insights with physical constraints.

Next-generation breakthroughs will emerge from integrated workflows combining high-throughput computations, automated experimental platforms, and reinforcement learning

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algorithms. The convergence of materials informatics, computational chemistry, and AI is dissolving traditional disciplinary boundaries. Quantum machine learning may redefine paradigms for electronic structure calculations, while topological data analysis tools could unveil global optimization pathways for material properties. Such interdisciplinary progress demands not only algorithmic innovation but also standardized systems for cross-domain knowledge representation.

The AI-driven theoretical reconfiguration of electrical materials science represents a revolutionary upgrade in human cognitive tools. From multidimensional correlation mining to cross-scale modeling, and from inverse design to autonomous experimentation, AI is redefining the epistemological dimensions and methodological frameworks of materials research. Future theoretical breakthroughs will transcend singular technological optimizations, instead focusing on human-AI collaborative paradigms: researchers contribute physical intuition and creative hypotheses, while AI navigates high-dimensional parameter spaces and deciphers complex systems. This symbiotic relationship may catalyze a "fourth paradigm" in materials science, unlocking unprecedented theoretical frontiers for performance breakthroughs and functional innovations in electrical materials.

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Reference：

[1] Liu Hengyu. Research on Properties of III-V Semiconductor Materials Based on Machine Learning [D], 2023.

[2] Wu Xiaoyu. Theoretical Prediction of Perovskite Defect States Based on Machine Learning [D], 2023.

[3] Hosseini ,et al. Machine Learning-enabled Prediction and Optimization of Hardness for Nb-Ti-V-Zr Refractory High Entropy Alloy [J]. Materials Today Communications, 2024, 40.

[4] Rao z, et al. Machine Learning-enabled High-entropy Alloy Discovery [Z]. arXiv, 2022.

[5]Zhao C, et al. Machine-learning for Designing Nanoarchitectured Materials by Dealloying [J]. Communications Materials, 2022, 3(1).

[6] Xu Jing, et al. Design of New Battery Materials Based on Big Data [J] Energy Storage Science and Technology [J]. 2024, 13(09): 2920-32.

[7] Deng B, et al. CHGNet as a Pretrained Universal Neural Network Potential for Charge-informed Atomistic Modelling [J]. Nature Machine Intelligence, 2023, 5(9): 1031-41.

[8] Lu C et al. Machine Learning: An Advanced Platform for Materials Development and State Prediction in Lithium-Ion Batteries [J]. Adv Mater, 2022, 34(25): 17.

[9] Cai ,et al. Prediction of Contact Resistance of Electrical Contact Wear Using Different Machine Learning Algorithms [J]. Friction, 2024, 12(6): 1250-71.

[10]Zhi shan,et al. Effect of Carbon Content on Hydrogen Resistance of Steel Materials Based on First-principles and Machine Learning [J] Journal of Metal Functional Materials [J]. 2024, 31(01): 44-50.

ISSN: 3029-1259 Vol.3,Issue 1 DOI: 10.12410/sia0201024

[11]Xu feng, et al.Estimation of P-S-N Curves of Metallic Materials Based on Bayesian Neural Network %J Journal of South China University of Technology (Natural Science Edition) [J]. 2023, 51(11): 82-92.

[12]Liu Shi, et al.Application of Machine Learning Potentials in Ferroelectric Material Research Acta Metallurgica Sinica [J]. 2024, 60(10): 1312-28.

[13]Don-Tsa et al. Predictive Models for Thermoelectric Properties of Inorganic Materials with Machine Learning [J]. Machine Learning-Science and Technology, 2024, 5(3).

[14]Yakushev A. Ensemble Regression Method for Predicting the Dependence of Electrical Resistance on the Elongation of Polymer Composite Materials [J]. Polymer Composites, 2024, 45(9): 8486-94.