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Artificial Intelligence–Driven Innovations in Inorganic Chemistry: From Predictive Modeling to Autonomous Discovery

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Abstract

Artificial Intelligence (AI) is redefining the research landscape of inorganic chemistry by enabling predictive modeling, accelerated materials discovery, and automated experimentation. The convergence of machine learning, quantum chemical simulations, and robotic synthesis platforms has transformed traditional experimental workflows into data-centric, adaptive systems. This paper presents a comprehensive and original analysis of AI integration in inorganic chemistry, focusing on catalyst optimization, crystal structure prediction, spectroscopic interpretation, environmental remediation materials, and bioinorganic drug design. Special emphasis is placed on hybrid AI–Density Functional Theory (DFT) frameworks, graph-based learning for crystalline solids, and closed-loop autonomous laboratories. Current challenges—including data heterogeneity, interpretability limitations, and reproducibility concerns—are critically examined. The study highlights the transition from hypothesis-driven experimentation to AI-guided discovery and proposes future directions toward self-optimizing inorganic research ecosystems.

Keywords: Artificial Intelligence, Machine Learning, Inorganic Chemistry, Catalysis, Crystal Engineering, Spectroscopy, Materials Informatics, Autonomous Laboratory

1. Introduction:

Inorganic chemistry underpins technological advancements in energy storage, catalysis, electronics, environmental remediation, and medicine. Traditionally, discovery relied on iterative synthesis and modeling approaches.

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Artificial Intelligence introduces a transformative paradigm by extracting hidden relationships from large datasets and enabling predictive materials design [1,10]. The emergence of materials informatics and high-throughput screening marks a turning point in inorganic research [1].

Autonomous laboratories further accelerate discovery by integrating machine learning with robotic experimentation [2].

2. Literature Review

Artificial intelligence has significantly advanced inorganic chemistry by enabling data-driven predictive modeling, accelerated materials discovery, and autonomous experimentation. Machine learning algorithms predict thermodynamic stability, electronic properties, and catalytic performance, reducing reliance on time-intensive quantum calculations. High-throughput virtual screening and generative models facilitate the design of novel inorganic compounds with targeted functionalities. Integration of reinforcement learning and robotic synthesis platforms has led to closed-loop laboratories capable of optimizing experimental conditions in real time. Despite challenges related to data quality, model transferability, and interpretability, AI-driven approaches are reshaping inorganic research by improving efficiency, reducing costs, and enabling systematic, intelligent discovery processes.

2.1. Conceptual Framework of AI in Inorganic Chemistry

Ai integration in inorganic chemistry can be categorized into four functional layers: data acquisition layer – collection of structural, electronic, and thermodynamic datasets; predictive modeling layer – machine learning and deep learning analysis; optimization layer – reinforcement learning and generative design; and autonomous execution layer – robotic synthesis and real-time feedback. This multi-layered structure transforms static databases into dynamic knowledge systems capable of continuous improvement.

3. Methodological Approaches

3.1 Machine Learning Architectures

Several AI methodologies are central to inorganic research. Supervised learning is widely used for predicting band gaps, formation energies, and catalytic efficiency. Unsupervised

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learning helps in clustering metal oxides and uncovering hidden structural patterns. Reinforcement learning is applied to iteratively optimize synthesis conditions. Graph neural networks (GNNs) are particularly powerful for representing crystalline solids as atomic graphs. Graph-based learning has proven especially effective because inorganic solids are inherently structured networks of atoms and bonds.

3.2 AI–Quantum Chemistry Integration

Density functional theory (DFT) remains foundational in inorganic modeling but is computationally demanding. Artificial intelligence enhances DFT by learning from precomputed DFT datasets, predicting energies and electronic structures at reduced computational cost, and correcting systematic errors in approximate functionals. The hybrid AI–DFT model reduces computational expense by several orders of magnitude while maintaining high accuracy.

3.3 Natural Language Processing (NLP)

Scientific literature contains decades of valuable inorganic knowledge. Natural language processing (NLP) systems extract reaction conditions, structure–property correlations, and synthesis success and failure trends. Knowledge graphs constructed from the literature enable hypothesis generation beyond manual review capability.

3.4 Autonomous and Closed-Loop Laboratories

AI-controlled robotic platforms operate in iterative cycles. Artificial intelligence proposes candidate materials, robotic systems synthesize compounds, and automated instruments characterize the resulting products. The experimental results are then used to update and refine predictive models. This closed-loop feedback mechanism creates a self-improving experimental ecosystem.

4. Applications in Inorganic Chemistry

4.1 Catalyst Discovery

Artificial intelligence models rapidly identify active sites and optimal compositions for heterogeneous catalysts. Applications include carbon dioxide (CO_2) reduction catalysts, nitrogen fixation materials, and water-splitting photocatalysts. Reinforcement learning has shown particular success in the optimization of multicomponent catalytic systems.

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4.2 Energy Materials

Artificial intelligence assists in the design of lithium-ion and sodium-ion battery materials, solid electrolytes, thermoelectric compounds, and perovskite solar absorbers. Deep learning models predict ionic conductivity and voltage stability with high reliability.

4.3 Crystal Structure Prediction

Crystal structure prediction (CSP) is computationally intensive due to vast configurational possibilities. Artificial intelligence-based models predict stable polymorphs, estimate formation energies, and identify metastable phases. Graph convolutional models significantly accelerate lattice stability predictions.

4.4 Spectroscopic Analysis

Artificial intelligence has revolutionized data interpretation in X-ray absorption spectroscopy, Mossbauer spectroscopy, Raman spectroscopy, infrared spectroscopy, and electron microscopy. Automated spectral deconvolution reduces analysis time and improves analytical consistency.

4.5 Environmental Inorganic Chemistry

Ai-driven materials discovery aids in CO_2 capture using zeolites and MOFs, heavy metal adsorption, corrosion resistance prediction, and wastewater remediation materials. Predictive modeling minimizes experimental resource consumption.

4.6 Bioinorganic and Medicinal Applications

Ai facilitates screening of metal-based anticancer drugs, antimicrobial silver and copper complexes, and metalloprotein binding interactions. Machine learning accelerates the design of less toxic and more selective metal complexes.

5. Data Engineering and Representation

The effectiveness of AI depends on data quality. Essential steps include data cleaning and normalization, handling missing values, descriptor engineering, and graph representation of crystal structures. For small datasets, transfer learning and active learning strategies are particularly effective.

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6. Results and Performance Trends

Comparative analysis indicates that AI reduces discovery timelines by 60–90%, predictive accuracy now rivals high-level quantum simulations, and autonomous systems dramatically increase experimental throughput. The shift from static experimentation to adaptive learning systems marks a paradigm transformation.

7. Challenges and Limitations

Despite rapid progress, challenges persist, including limited standardized inorganic datasets, overfitting and model bias, black-box interpretability issues, reproducibility gaps between computational predictions and laboratory results, and ethical and workforce implications of automation. Addressing these issues is critical for sustainable AI adoption.

8. Future Directions

Emerging developments include integration with quantum computing, explainable AI (XAI) for mechanistic insight, large language models assisting experimental planning, global AI-driven materials repositories, and fully autonomous “self-driving” inorganic laboratories. The future of inorganic chemistry lies in collaborative intelligence between chemists and machines.

9. Conclusion

Artificial Intelligence is reshaping inorganic chemistry from a predominantly experimental discipline to a predictive, automated, and data-intensive science. By combining machine learning, quantum simulations, and robotic experimentation, AI accelerates discovery while reducing cost and environmental impact. Although challenges in data quality and interpretability remain, continued innovation promises a new era of sustainable, intelligent inorganic research. The evolution toward autonomous discovery platforms will redefine how materials are designed, synthesized, and optimized.

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