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Role of Machine Learning in Inorganic and Coordination Chemistry: Applications and Challenges

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Abstract

Machine learning (ML) is a branch of artificial intelligence. ML is revolutionizing various areas of chemistry by enhancing predictions of chemical properties, uncovering hidden patterns in complex data, and accelerating the discovery of new compounds. Machine learning is also accelerating research and development in the complex and limited data fields of coordination and inorganic chemistry. This paper examines the advancements in inorganic and coordination chemistry enabled by the application of ML. These advancements include the prediction of chemical properties, the design of effective catalysts, spectroscopy, and the analysis of compound structures. This paper discusses case studies where ML techniques are effectively applied to research and development in inorganic and coordination chemistry. In the end of this paper, the key challenges in the path of using ML techniques in fostering innovation in inorganic and coordination chemistry are highlighted.

Keywords: ML, inorganic chemistry, coordination chemistry, property prediction, catalyst design, spectroscopy, data scarcity, model interpretability.

1. Introduction

Inorganic and coordination chemistry are the main branches of chemistry. Inorganic and coordination chemistry deal with the synthesis, behaviour analysis, and their industrial applications. These inorganic and coordination compounds and complexes play significant roles in catalyst design, materials science, bioinorganic processes, and various industrial applications. However, theoretical predictions and experimental characterization of inorganic compounds and coordination complexes are challenging and resource-intensive due to their structural complexity and diverse bonding characteristics. To address these challenges, the research community has suggested using machine learning (ML) techniques to foster innovation in inorganic and coordination chemistry in literature [1, 2].

ML is a branch of artificial intelligence. ML techniques enable computers to learn patterns from data and make predictions or decisions without requiring explicit programming. It encompasses a range of algorithms, including supervised, unsupervised, and reinforcement learning. ML utilizes data-driven approaches to model complex and nonlinear relationships in chemical systems. These data-driven approaches do not rely on explicit physical reactions and equations. These characteristics of machine learning algorithms make them valuable tools for understanding and predicting chemical behaviour in inorganic and coordination chemistry [3,4].

ML has achieved significant success in organic chemistry, drug development, and materials informatics. ML also has excellent potential in inorganic and coordination chemistry in terms of innovation and research advancement. It can help by addressing computational challenges, accurately predicting chemical properties, and guiding experimental synthesis. However, datasets in inorganic and coordination chemistry are typically smaller and more diverse than those in organic chemistry. Therefore, careful data collection, practical feature analysis engineering, and rigorous model validation are essential for applying ML in inorganic and coordination chemistry [5,6].

ML methods utilize chemical descriptors, structural data, and experimental results to train predictive or generative models.

- Supervised learning relates input features (e.g., molecular descriptors) to target properties (e.g., stability, band gap)
- Unsupervised learning uncovers hidden structures and groups within unlabelled chemical datasets.
- Semi-supervised learning leverages limited labelled chemical data alongside abundant unlabelled data to enhance prediction performance with minimal manual labelling effort.
- Reinforcement learning is emerging as a tool for reaction planning and synthesis optimization.

Neural networks and deep learning techniques fall under the broader umbrella of machine learning. In inorganic and coordination chemistry, neural networks and deep learning also aid in predicting properties, interpreting data, and accelerating the design of novel compounds and catalysts.

This paper reviews the role of ML in advancing research and discovery in inorganic and coordination chemistry. This paper outlines ML applications, categorizes state-of-the-art methods, discusses relevant case studies, and highlights key challenges and future research directions.

2. Applications in Inorganic and Coordination Chemistry

2.1. Property Prediction

Predicting physicochemical properties is fundamental for catalyst design, materials selection, and process optimization. ML models have been developed to predict:

- **Thermodynamic stability:** For example, kernel ridge regression and graph neural networks can predict formation energies of metal oxides and perovskites [7, 8 ,9].
- **Electronic structure:** Models can approximate HOMO-LUMO gaps, redox potentials, and spin states [10,11,12].
- **Magnetic properties:** Supervised ML predicts exchange coupling constants in transition metal complexes [13,14, 15].

These predictions aid rapid screening and reduce reliance on expensive quantum mechanical calculations.

2.2. Catalyst Design

Coordination complexes are vital homogeneous catalysts for industrial and environmental processes. ML facilitates:

- **Ligand design:** Generative models propose ligands that stabilize desired metal oxidation states [16,17,18].
- **Reaction pathway prediction:** ML-based reaction network analysis identifies low-energy pathways [19, 20, 21].

- **Activity and selectivity estimation:** Predictive models correlate structural features with catalytic performance [22,23,24].

Recent studies integrate active learning to refine models using new experimental data iteratively.

2.3. Spectroscopic Analysis

Spectroscopy (X-ray, NMR, EPR) is essential for characterizing coordination compounds. ML enhances spectroscopy by:

- Predicting spectral features from structural data [25,26,27].
- Automating interpretation of complex spectra [28,29,30].
- Reducing noise and improving resolution through data denoising algorithms [31, 32,33].

Notably, ML models have been trained on X-ray absorption spectroscopy datasets to predict oxidation states and local environments of metal centres.

2.4. Structural Elucidation and Data Mining

Predicting and visualizing structures of coordination complexes is challenging due to flexible geometries and multiple isomers. ML techniques contribute to:

- Crystal structure prediction [34,35, 36].
- Identifying patterns in crystallographic databases [37, 38, 39].
- Clustering compounds with similar structural motifs [40,41,42].

Graph neural networks have shown promise in learning from 3D molecular graphs to predict feasible coordination geometries.

3. Case Studies

3.1. DeepMind's GNoME

DeepMind's Graph Networks for Materials Exploration (GNoME) project uses graph neural networks to predict stability and synthesize new inorganic crystals, including complex oxides and perovskites, accelerating materials discovery by orders of magnitude [43].

3.2. ML for Spin Crossover Complexes

Spin crossover (SCO) complexes exhibit switchable spin states, which are relevant in sensors and memory devices. ML models using decision trees and neural networks have predicted transition temperatures and hysteresis behaviours, guiding experimental synthesis [44, 45].

3.3. Spectral Prediction for Transition Metals

XANESNET, an ML framework, predicts X-ray absorption near edge structure (XANES) spectra for transition metal complexes, enabling rapid screening of oxidation states and coordination environments [46, 47].

4. Challenges

Despite remarkable progress, several challenges hinder widespread ML adoption in inorganic and coordination chemistry.

4.1. Data Scarcity and Quality

Unlike organic molecules, large, standardized datasets for inorganic compounds are rare. Experimental data is scattered across publications, with inconsistent formats and missing metadata. This limits model accuracy and generalizability.

4.2. Feature Representation

Capturing essential chemical information is nontrivial. Descriptors must encode electronic, steric, and geometric features unique to metal centres and ligands. Graph-based methods partially address this issue, but can struggle with d-electron effects.

4.3. Model Interpretability

Black-box ML models provide limited mechanistic insight, which is crucial for chemists. There is a growing demand for explainable AI (XAI) approaches that reveal structure-property relationships.

4.4. Integration with Quantum Chemistry

Hybrid methods that combine ML and quantum mechanics promise both accuracy and speed. However, integrating machine learning corrections with ab initio methods while ensuring physical consistency remains a significant challenge.

4.5. Generalization and Transferability

Models trained on narrow chemical spaces may fail when applied to novel metal-ligand combinations. Transfer learning and domain adaptation techniques are under exploration.

5. Future Directions

To harness ML's full potential in inorganic and coordination chemistry, the community should pursue:

- **Open, high-quality datasets:** Collaborative initiatives to standardize data collection and sharing will improve reproducibility.
- **Interpretable models:** Development of ML architectures that align with chemical principles and offer explainable predictions.
- **Automated synthesis and feedback loops:** Coupling ML predictions with robotic synthesis for closed-loop discovery.
- **Integration with quantum chemical workflows:** Seamless hybrid modelling pipelines for accurate and efficient predictions.
- **Interdisciplinary training:** Chemists should gain familiarity with machine learning (ML) concepts, while data scientists learn relevant chemical knowledge.

6. Conclusion

Machine learning is poised to transform inorganic and coordination chemistry by enabling rapid and accurate predictions, as well as guiding experimental design. While challenges persist—chiefly related to data limitations, interpretability, and transferability—ongoing advances in algorithms, data curation, and interdisciplinary collaboration promise to address these barriers. This evolving synergy between machine learning and chemistry holds the key to accelerated discovery of novel materials, catalysts, and functional complexes, shaping the future of chemical research and industrial applications.

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