PHOTOLUMINESCENCE RESEARCH POWERED BY ARTIFICIAL INTELLIGENCE: FROM SPECTRAL ANALYSIS TO MATERIALS DISCOVERY- A MINI REVIEW

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Abstract

Photoluminescence (PL) spectroscopy is a widely used technique for characterizing optoelectronic and luminescent materials. However, conventional PL spectral interpretation is often time-consuming and limited by human-dependent analysis, especially for large and complex datasets. The emergence of artificial intelligence (AI) and machine learning (ML) has transformed materials science by enabling automated spectral interpretation, pattern recognition, and accelerated materials discovery. In particular, ML-based models such as support vector machines (SVM), random forest (RF), and artificial neural networks (ANN) have demonstrated high accuracy in predicting material properties and classifying photoluminescence spectra. This review summarizes recent advances in AI-driven PL research, focusing on spectral analysis, defect identification, temperature-dependent PL behaviour, and AI-assisted materials discovery. The integration of AI with PL spectroscopy enables faster, more accurate, and data-driven exploration of luminescent materials for next-generation optoelectronic applications.

Keywords: Photoluminescence; artificial intelligence; machine learning; optoelectronics; luminescent materials.

1. Introduction

Photoluminescence (PL) is the emission of light from a substance after it has absorbed electromagnetic radiation, often in the ultraviolet or visible area of the spectrum. When photons strike a material, electrons absorb the incident energy and transition from the valence band or ground electronic state to a higher-energy excited state. These excited electrons are unstable and eventually return to their lower-energy state, releasing excess energy as light[1]. The wavelength and intensity of the emitted radiation depend on the electronic structure and chemical composition of the material. The photoluminescence process mainly involves two important mechanisms: fluorescence and phosphorescence[2]. In fluorescence, the emitted light is released rapidly, usually within nanoseconds after excitation, whereas phosphorescence occurs more slowly because the excited electrons remain trapped in metastable energy states before radiative relaxation[3]. The distinction between these two mechanisms is important in understanding the optical behaviour of organic molecules, semiconductors, phosphor materials, and nanostructured systems. PL spectroscopy has become a valuable characterization technique because it provides detailed information about the optical and electronic properties of materials[4]. It is commonly employed to investigate band-gap energy, impurity levels, crystal defects, charge-carrier recombination, and energy transfer mechanisms. In semiconductor and nanomaterial research, photoluminescence analysis helps evaluate material quality, structural uniformity, and defect concentrations without causing damage to the sample. Due to its high sensitivity, simplicity, and non-destructive nature, PL analysis is extensively used in physics, chemistry, materials science, and optoelectronic engineering[5]. PL spectroscopy is recognized as one of the most effective analytical

techniques for investigating the optical and electronic behaviour of a wide variety of materials. The method is based on the interaction between incident light and the electronic structure of a substance, allowing researchers to obtain detailed information regarding energy transitions, defect states, and recombination pathways. Because the emitted luminescence is directly related to the internal electronic configuration of a material, PL analysis serves as a powerful tool for understanding the fundamental physicochemical properties of semiconductors, nanostructures, polymers, biomaterials, and hybrid composites. Even a very small concentration of defects, vacancies, or dopant atoms can significantly influence the PL emission spectrum. As a result, PL measurements are widely used to evaluate crystal quality, defect density, and impurity levels in semiconductors and thin-film materials. In nanomaterials such as quantum dots and metal oxide nanoparticles, PL behaviour provides important insights into quantum confinement effects, particle size distribution, surface states, and excitonic interactions[6].

Another significant feature of PL spectroscopy is its non-destructive nature. Unlike several conventional characterization techniques that may require complex sample preparation or cause physical damage to the material, PL measurements can often be performed rapidly and without altering the sample structure[7]. This advantage makes PL particularly suitable for fragile biological samples, organic compounds, and advanced nanostructured systems. Additionally, the technique can be carried out over a broad temperature range, enabling researchers to study temperature-dependent electronic transitions and charge carrier dynamics[8]. PL spectroscopy also plays an essential role in the development of modern optoelectronic and photonic devices. It is extensively applied in the characterization of light-emitting diodes (LEDs), laser diodes, photodetectors, solar cells, and photocatalytic materials. By analysing emission intensity, peak position, and lifetime characteristics, researchers can optimize material performance for improved energy conversion and light-emission efficiency. Furthermore, time-resolved photoluminescence techniques are commonly used to investigate electron–hole recombination rates and carrier lifetimes in photovoltaic and semiconductor materials[9].

In recent years, photoluminescence analysis has gained increasing importance in biomedical and environmental applications. Fluorescent nanoparticles and quantum dots exhibiting strong PL properties are widely employed in bioimaging, biosensing, drug delivery, and disease diagnostics due to their high brightness and excellent sensitivity. PL-based sensing systems are also used for detecting toxic metal ions, organic pollutants, and hazardous chemicals in environmental monitoring studies. The versatility, rapid response, and high analytical precision of photoluminescence techniques continue to expand their importance across multiple scientific disciplines[10].

PL plays a crucial role in modern scientific research and technological development due to its wide applicability across multiple advanced fields. In semiconductor technology, PL is extensively used for evaluating material quality during device fabrication, especially in thin films, heterostructures, and epitaxial layers[11]. It helps in identifying defects, impurities, and recombination centres that directly influence device performance. In optoelectronic devices such as LEDs and laser diodes, PL studies are used to optimize emission efficiency, band alignment, and carrier recombination processes, which are essential for improving brightness, stability, and energy efficiency of these devices[12]. In photovoltaic research, photoluminescence is an important diagnostic tool for solar cell materials. It provides insights into bandgap properties, non-radiative recombination losses, and charge carrier lifetime, which are key factors affecting solar energy conversion efficiency. By analysing PL emission characteristics, researchers can identify material limitations and improve the design of high-performance solar cells, including perovskite-based and thin-film solar technologies[13].

In nanotechnology, PL spectroscopy is fundamental for understanding the optical behaviour of nanomaterials such as quantum dots, nanowires, and metal oxide nanoparticles. The emission properties of these materials

strongly depend on particle size, shape, and surface chemistry. This size-dependent emission phenomenon, known as quantum confinement, is widely studied using PL techniques to develop tuneable light-emitting materials for display technologies, bio-labelling, and advanced photonic systems[14].

PL also has significant applications in biosensing and biomedical imaging. Fluorescent nanomaterials and organic dyes with strong PL properties are used as probes for imaging cells, tissues, and biological processes at the molecular level. These PL-based probes offer high spatial resolution and sensitivity, making them suitable for early disease detection, cancer imaging, and real-time tracking of biological interactions[15]. In environmental science, PL-based sensors are widely used for detecting hazardous substances such as heavy metal ions, toxic gases, and organic pollutants in water and air systems. These sensors offer rapid response times, high selectivity, and excellent sensitivity, making them effective for real-time environmental monitoring and pollution control. Additionally, PL techniques are used in photocatalysis research to study charge separation efficiency and degradation mechanisms of pollutants under light irradiation[16,17].

To identify the patterns automatically from the data, machine learning uses collection of techniques.Machine learning has been widely used in discovery and design of new materials in materials science. In the past, the research and development of optoelectronic materials needed a lot of experimental efforts and time. However, with the development of computational methods, the prediction of material structures and properties has become easier, faster and more efficient. The combination of artificial intelligence with photoluminescence (PL) analysis is one of the latest and most important advances in spectrum interpretation and materials optimization.AI-based methods have the potential to revolutionize the discovery of materials, but the dependence on large datasets and the challenges of model validation emphasize the need for a balanced approach that integrates artificial intelligence with traditional experimental methodologies[18,19].

According to a review of the literature, artificial intelligence applications in photoluminescence spectroscopy are still in their infancy and have not received much attention. In this regard, the present review concentrates on examining and summarizing the new AI-driven methods and computational tools used in this field, which range from sophisticated spectral analysis methods to expedited materials characterization and discovery.

2. Fundamentals of Photoluminescence Spectroscopy

PL spectroscopy is an important optical characterization technique used to study the electronic and optical properties of materials. In PL spectroscopy, a material absorbs photons from an external light source and subsequently re-emits light through radiative recombination processes. The emitted light provides valuable information regarding the band structure, defect states, impurity levels, carrier dynamics, and energy transitions present within the material. PL analysis is widely applied in semiconductors, nanomaterials, quantum dots, thin films, and luminescent compounds due to its non-destructive and highly sensitive nature[20].

The basic principle of PL involves three major processes: excitation, relaxation, and emission. During excitation, incident photons with sufficient energy promote electrons from the valence band to the conduction band or from the ground state to an excited state. The excited electrons then undergo non-radiative relaxation toward lower energy states before recombining with holes and emitting photons. The wavelength and intensity of the emitted light depend on the electronic structure and chemical environment of the material[21]. A typical PL spectroscopy setup consists of a light excitation source, monochromators, sample holder, detector, and data acquisition system. Lasers and xenon lamps are commonly used as excitation sources because they provide high-intensity radiation over a wide wavelength range. The emitted light from the sample is dispersed using monochromators and detected by photomultiplier tubes (PMTs) or charge-coupled devices (CCDs). The resulting PL spectrum represents emission intensity as a function of wavelength or photon energy[22,23].

PL spectroscopy can be categorized into steady-state PL and time-resolved PL techniques. Steady-state PL measures the overall emission characteristics under continuous excitation, while time-resolved PL evaluates the decay lifetime of excited carriers after pulsed excitation. Time-resolved studies are particularly useful for understanding recombination kinetics,carrier trapping, and defect-assisted transitions in semiconductors and nanostructures[24]. The PLemission process generally occurs through fluorescence or phosphorescence mechanisms. Fluorescence involves rapid radiative transitions from singlet excited states and usually occurs within nanoseconds. Phosphorescence involves transitions through triplet states and exhibits longer emission lifetimes due to spin-forbidden transitions. These emission behaviours help in understanding molecular interactions and energy transfer processes in luminescent systems[25]. In semiconductor materials, PL spectroscopy is extensively employed to determine band gap energy, crystal quality, impurity concentration, and defect density. Variations in peak position, peak width, and emission intensity provide direct insight into structural imperfections and electronic states. Temperature-dependent PL measurements are also used to study exciton behaviour, thermal quenching, and carrier localization effects[26]. Nanomaterials and quantum-confined systems exhibit unique PL properties due to size-dependent electronic transitions. Quantum dots, nanoparticles, and two-dimensional materials often show tuneable emission wavelengths and enhanced luminescence efficiency. PL spectroscopy therefore plays a significant role in nanotechnology, biosensing, photocatalysis, and optoelectronic device development[27].

Recent advancements in computational methods and artificial intelligence have expanded the capabilities of PL spectroscopy. Machine learning algorithms are increasingly used for automated spectral interpretation, defect classification, and prediction of material properties from PL data. The integration of AI with PL analysis enables rapid processing of large datasets and accelerates the discovery of advanced luminescent materials.

3. Artificial Intelligence and Machine Learning Techniques in Materials Science

AI and ML have emerged as transformative tools in materials science, enabling rapid data analysis, prediction of material properties, and accelerated discovery of advanced functional materials. Traditional experimental approaches in materials research are often expensive and time-consuming, whereas AI-driven methods can analyse large datasets efficiently and identify hidden relationships between structure, composition, and performance. These computational approaches are increasingly applied in semiconductors, nanomaterials, catalysts, batteries, polymers, and optoelectronic systems[28].

ML is a subset of AI that enables computer systems to learn patterns from data without explicit programming. In materials science, ML algorithms are trained using experimental or computational datasets to predict material behaviour and optimize performance. The major categories of ML include supervised learning, unsupervised learning, and reinforcement learning. Supervised learning uses labelled datasets for prediction and classification tasks, while unsupervised learning identifies hidden patterns or clustering within unlabelled data[29].

Support Vector Machine (SVM) is one of the widely used supervised learning techniques in materials research. SVM models are effective for classification and regression problems because they can handle nonlinear relationships and high-dimensional datasets. In spectroscopy and semiconductor studies, SVM algorithms are frequently used for phase identification, defect classification, and spectral interpretation with high accuracy.Random Forest (RF) is another important ML algorithm extensively used in materials informatics. RF operates through multiple decision trees and combines their outputs to improve prediction accuracy and reduce overfitting. The method is particularly useful for predicting thermal stability, conductivity, optical behaviour, and crystal structure-property relationships in complex materials systems[30].

Artificial Neural Networks (ANNs) are computational models inspired by the structure and function of biological neural systems. ANNs consist of interconnected nodes capable of learning complex nonlinear relationships

from large datasets. In materials science, ANNs are employed for predicting band gap energy, luminescence behaviour, mechanical properties, and synthesis optimization. Their capability to process multidimensional data makes them highly valuable for spectroscopy and materials discovery applications[31,32].

Deep learning, an advanced branch of machine learning, utilizes multilayer neural networks for automated feature extraction and complex data analysis. Convolutional Neural Networks (CNNs) are commonly used for image-based materials characterization, microscopy analysis, and spectral pattern recognition. Recurrent Neural Networks (RNNs) are also applied in sequential data processing and time-dependent material behaviour analysis[33,34].

AI-driven materials informatics integrates computational databases, high-throughput screening, and ML algorithms to accelerate materials discovery. Large materials databases such as the Materials Project and Open Quantum Materials Database provide extensive datasets for training predictive models. These platforms enable researchers to identify promising materials with targeted optical, electronic, and structural properties before experimental synthesis[35].

Feature engineering plays a critical role in ML-based materials research. Material descriptors such as atomic radius, electronegativity, crystal symmetry, and electronic structure parameters are used as input features for predictive models. Proper feature selection improves model accuracy and enhances interpretation of structure-property relationships[36]. AI techniques are increasingly integrated with spectroscopic methods such as PL, Raman spectroscopy, infrared spectroscopy, and X-ray diffraction. ML-assisted spectral analysis enables automated peak detection, defect identification, noise reduction, and classification of complex spectral datasets. These methods significantly reduce manual interpretation time and improve analytical precision[37,38].

Despite significant progress, challenges remain in AI-based materials science, including limited availability of high-quality datasets, data inconsistency, model interpretability, and computational cost. Explainable AI and hybrid physics-informed machine learning models are being developed to improve reliability and scientific understanding of predictions. Continued advancements in AI are expected to revolutionize materials design, characterization, and industrial applications in the future.AIhas significantly improved the efficiency and accuracy of PL spectral analysis by enabling automated interpretation of complex spectral datasets. Conventional PL analysis often requires manual peak fitting, defect identification, and spectral comparison, which can be time-consuming and susceptible to human error. AI-driven computational methods provide rapid data processing, pattern recognition, and predictive analysis, thereby enhancing the understanding of luminescent materials and optoelectronic systems[39,40].

4. Machine Learning and Deep Learning for PL Characterization

ML and DL techniques have become powerful tools for PL characterization, offering rapid and automated analysis of complex spectral data. Conventional PL interpretation often relies on manual peak fitting and expert judgement, which can be labour-intensive and less effective for large datasets. ML and DL methods improve the efficiency of PL characterization by enabling automatic feature extraction, classification, prediction, and pattern recognition from spectral information[41,42,43,44].

Supervised machine learning algorithms are commonly employed for analysing PL spectra because they can learn relationships between spectral features and material properties. By training on labelled datasets, these algorithms can predict emission characteristics, identify luminescent phases, and classify semiconductor materials with high precision. Suchapproaches are widely used in nanomaterial and optoelectronic research[45]. K-nearest neighbour (KNN) algorithms have shown effectiveness in PL spectral classification due to their simplicity and strong pattern recognition capability. KNN methods compare unknown spectra with known reference datasets to determine similarities in emission behaviour. These algorithms are useful in distinguishing luminescent materials and identifying spectral variations caused by defects or impurities[46].

Decision tree-based learning methods are also applied in PL characterization for spectral categorization and property prediction. These models generate interpretable decision pathways based on spectral intensity, wavelength position, and emission features[47].

Decision tree approaches are valuable for identifying key parameters influencing luminescence performance techniques provide advanced capabilities for handling large and multidimensional PL datasets. Unlike traditional ML algorithms, deep neural networks can automatically learn hierarchical spectral features without extensive manual preprocessing. This enables more accurate analysis of nonlinear spectral relationships and complex emission behaviours in advanced materials systems[48].

Convolutional Neural Networks (CNNs) are widely used in PL characterization because of their strong feature extraction ability. CNN models can analyse spectral images and multidimensional PL maps to detect hidden patterns related to defects, excitonic transitions, and crystal quality. These techniques are particularly effective in high-throughput characterization of semiconductor nanostructures[49].

Autoencoder-based deep learning models are increasingly used for denoising and dimensionality reduction in PL spectroscopy. These unsupervised learning methods compress spectral information into lower-dimensional representations while preserving important features. Such approaches improve signal quality and enhance the interpretation of weak luminescence signals[50,51].

Recurrent Neural Networks (RNNs) and Long Short-Term Memory (LSTM) models are useful for studying time-dependent PL behaviour and dynamic carrier recombination processes. These algorithms can process sequential spectral data and predict temporal changes in luminescence intensity under varying experimental conditions. Deep learning methods are also contributing to autonomous materials characterization systems. Integration of AI with PL instrumentation enables real-time spectral acquisition, automated interpretation, and rapid optimization of synthesis conditions. Such intelligent characterization platforms are expected to accelerate the development of advanced luminescent and optoelectronic materials[52,53].

5. AI-Driven Materials Discovery

AI has emerged as a powerful approach for accelerating materials discovery by enabling rapid prediction, screening, and optimization of material properties. Traditional materials development often requires extensive experimental trials and computational simulations, which consume significant time and resources. AI-driven methods can analyse vast datasets, identify hidden trends, and predict promising material candidates with improved efficiency, thereby transforming the conventional materials research process[54]. Machine learning algorithms are widely employed to establish relationships between material composition, structure, and functional properties. These algorithms learn from experimental and theoretical databases to predict characteristics such as band gap energy, thermal conductivity, luminescence efficiency, and mechanical strength. Such predictive modelling significantly reduces the need for repeated laboratory experiments[55].

High-throughput computational screening combined with AI has become an effective strategy for discovering advanced materials. In this approach, thousands of possible compounds are computationally evaluated using predictive algorithms to identify candidates with desirable properties. This method is particularly valuable in the development of semiconductors, photovoltaic materials, catalysts, and battery systems[56,57]. Natural language processing (NLP), another branch of AI, is increasingly used in materials research for extracting scientific knowledge from published literature. NLP systems can automatically analyse research articles, identify synthesis methods, and summarize material-property relationships, thereby assisting researchers in discovering trends and unexplored research areas[58]. Generative AI models are gaining importance in the design of new materials with targeted properties. These models can propose hypothetical molecular or crystal structures based on desired performance criteria, enabling inverse materials design. This approach is particularly useful for discovering high-efficiency phosphors, catalysts, and functional nanomaterials[59,60].

6. Challenges and Limitations

Challenges

Although AI has significantly advanced PL research, several challenges still limit its full potential. One major issue is the lack of large, standardized, and high-quality PL datasets. PL spectra often vary due to differences in instrumentation, excitation sources, and sample preparation, making it difficult to build universal models that generalize across laboratories and material systems. A further challenge is the limited interpretability of machine learning and deep learning models. Many AI methods, especially deep neural networks, act as black boxes, making it difficult to understand how spectral features are linked to physical processes such as defect states, recombination mechanisms, or band gap transitions. This reduces scientific trust in AI-driven predictions.Transferability of AI models across different materials systems are also a major challenge. A model trained on one class of materials e.g., quantum dots may not perform well on another e.g., wide-bandgap semiconductors due to fundamentally different emission mechanisms and spectral features. This limits the universal applicability of trained models. Integration of AI with experimental PL spectroscopy systems remains technically challenging. Real-time spectral acquisition, data preprocessing, and model inference require well-coordinated hardware–software frameworks. Lack of standardized pipelines slows down the adoption of AI in routine PL laboratories.

Limitations

The dependence of AI models on large training datasets is limitation in PL research. In many materials systems, especially emerging nanomaterials and novel semiconductors, experimental PL data is scarce. This data scarcity restricts model performance and increases the risk of overfitting, where models perform well on training data but poorly on unseen samples. Another important limitation is data inconsistency and noise in experimental PL spectra. Variations such as baseline drift, spectral overlap, and instrumental artifacts can significantly affect model training and prediction accuracy. Without proper preprocessing and normalization, AI models may learn misleading patterns rather than true physical relationships. Computational cost is another limitation, particularly for deep learning models used in high-resolution PL spectral analysis and materials screening. Training complex neural networks requires significant computational resources, including GPUs and high-performance computing systems, which may not be accessible to all research groups. Another limitation is the difficulty in capturing physical laws within purely data-driven models. While AI can identify correlations in PL spectra, it may not always respect underlying quantum mechanical principles such as selection rules, exciton dynamics, or recombination pathways. This can lead to physically inconsistent predictions. Finally, ethical and reproducibility concerns are emerging in AI-assisted materials research. Lack of transparency in model development, incomplete reporting of training datasets, and inconsistent evaluation metrics can lead to irreproducible results. Establishing standardized reporting protocols is essential for reliable scientific progress.

7. Future Perspectives

The future of PL research is expected to be strongly influenced by AI, particularly through the development of more robust, generalizable, and physics-aware models. Integration of AI with PL spectroscopy will likely move beyond simple spectral classification toward comprehensive understanding of electronic transitions, defect physics, and energy transfer mechanisms in complex materials. A major future direction is the development of physics-informed machine learning (PIML) models that incorporate fundamental physical laws into data-driven frameworks. Such approaches can improve model reliability by ensuring consistency with quantum mechanical principles, exciton dynamics, and radiative recombination processes observed in PL systems. Another promising direction is the creation of large, standardized, and open-access PL spectral databases. These datasets will enable more accurate training of machine learning models and improve reproducibility across laboratories. Global data-sharing initiatives are expected to play a key role in advancing AI-driven PL research. Future PL systems are likely to incorporate real-time AI-assisted spectral acquisition and analysis. Intelligent spectroscopy platforms will enable automated peak detection, noise correction, and defect identification during experiments, significantly reducing analysis time and improving

experimental efficiency. Deep learning architectures such as convolutional neural networks CNNs and transformer-based models are expected to become more widely used for PL spectral interpretation. These models can extract complex hierarchical features from spectral and imaging data, enabling improved classification of luminescent materials and defect states. Generative AI models will play an increasingly important role in inverse design of luminescent materials. These models can propose new compounds with desired emission wavelengths, quantum efficiencies, and thermal stability, thereby accelerating the discovery of next-generation phosphors and optoelectronic materials. The combination of AI with high-throughput experimental platforms and robotics will lead to fully autonomous self-driving laboratories for PL-based materials discovery. These systems will be capable of performing experiments, analysing spectra, and optimizing synthesis conditions with minimal human intervention.

8. Conclusion

PL spectroscopy remains a powerful and versatile technique for investigating the optical and electronic properties of a wide range of materials, including semiconductors, nanostructures, and luminescent compounds. Its ability to provide detailed insights into band structure, defect states, carrier recombination, and energy transfer processes makes it an essential tool in modern materials science and optoelectronic research. In recent years, the integration of AI and ML with PL analysis has significantly enhanced data interpretation, spectral analysis, and materials discovery. AI-based approaches enable automated processing of complex spectral datasets, improve accuracy in defect identification, and accelerate the prediction of material properties. Furthermore, advanced techniques such as deep learning, physics-informed models, and high-throughput data-driven frameworks are expanding the scope of PL spectroscopy from conventional analysis to intelligent and autonomous materials characterization. Despite these advancements, challenges such as limited high-quality datasets, model interpretability, transferability issues, and integration with experimental systems still need to be addressed. However, ongoing developments in explainable AI, standardized databases, and self-driving laboratories are expected to overcome these limitations in the future.

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